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Science & Technology Review

Lawrence Livermore National Laboratory

Contents

Featured Articles

Introduction

Thank you for your interest in the activities of the Lawrence Livermore National Laboratory Computation Directorate. This collection of articles from the Laboratory's Science & Technology Review highlights the most significant computational projects, achievements, and contributions during 2002.

In 2002, LLNL marked the 50th anniversary of its founding. Scientific advancement in support of our national security mission has always been the core of the Laboratory. So that researchers could better under and predict complex physical phenomena, the Laboratory has pushed the limits of the largest, fastest, most powerful computers in the world.

In the late 1950's, Edward Teller - one of the LLNL founders - proposed that the Laboratory commission a Livermore Advanced Research Computer (LARC) built to Livermore's specifications. He tells the story of being in Washington, DC, when John Von Neumann asked to talk about the LARC. He thought Teller wanted too much memory in the machine. (The specifications called for 20-30,000 words.) Teller was too smart to argue with him. Later Teller invited Von Neumann to the Laboratory and showed him one of the design codes being prepared for the LARC. He asked Von Neumann for suggestions on fitting the code into 10,000 words of memory, and flattered him about "Labbies" not being smart enough to figure it out. Von Neumann dropped his objections, and the LARC arrived with 30,000 words of memory. Memory, and how close memory is to the processor, is still of interest to us today.

Livermore's first supercomputer was the Remington-Rand Univac-1. It had 5600 vacuum tubes and was 2 meters wide by 4 meters long. This machine was commonly referred to as a 1 KFlop machine [E+3].)

Skip ahead 50 years. The ASCI White machine at the Laboratory today, produced by IBM, is rated at a peak performance of 12.3 TFlops or E+13. We've improved computer processing power by 10 orders of magnitude in 50 years, and I do not believe there's any reason to think we won't improve another 10 orders of magnitude in the next 50 years. For years I have heard talk of hitting the physical limits of Moore's Law, but new technologies will take us into the next phase of computer processing power such as 3-D chips, molecular computing, quantum computing, and more.
Big computers are icons or symbols of the culture and larger infrastructure that exists at LLNL to guide scientific discovery and engineering development. We have dealt with balance issues for 50 years and will continue to do so in our quest for a digital proxy of the properties of matter at extremely high temperatures and pressures.

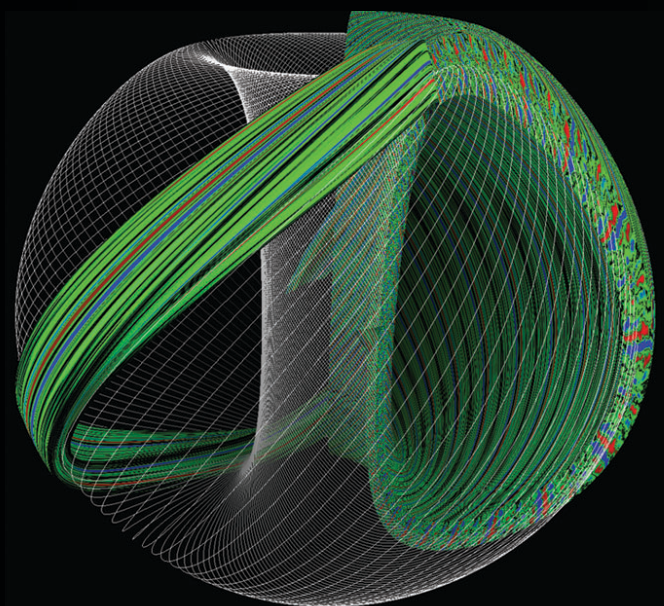
I believe that the next big computational win will be the merger of high-performance computing with information management. We already create terabytes - soon to be petabytes - of data. Efficiently storing, finding, visualizing and extracting data and turning that into knowledge which aids decision-making and scientific discovery is an exciting challenge.

In the meantime, please enjoy this retrospective on computational physics, computer science, advanced software technologies, and applied mathematics performed by programs and researchers at LLNL during 2002. It offers a glimpse into the stimulating world of computational science in support of the national missions and homeland defense.

Dona L. Crawford is the associate director for the Lawrence Livermore National Laboratory Computation Directorate.

Simulating Turbulence in Magnetic Fusion Plasmas

Microturbulence, a long-time nemesis of magnetic fusion energy experiments, is being understood in unprecedented detail thanks to new three-dimensional simulations.



This Livermore simulation shows a magnetic field line (white) wrapping around a torus, or doughnut-shaped configuration of plasma. Magnetic field lines are embedded within the plasma, with individual particles traveling along each field line. The color contours indicate microturbulent fluctuations in the plasma density. Regions with similar density—microturbulent eddies indicated by regions of similar color—stretch along the field lines, while varying rapidly across the field lines. These microturbulent eddies transport heat from the plasma's superhot core to the cold outer edge.

SINCE the 1950s, Lawrence Livermore has been one of the world's leading centers of magnetic fusion energy research. Magnetic fusion uses intense magnetic fields to confine an extremely hot gas of electrons and positively charged ions called a plasma. Under the right conditions, the plasma ions undergo fusion reactions, the energy source of the Sun and other stars.

The long-standing goal of fusion researchers has been to duplicate the cosmos's means of producing energy to provide a virtually inexhaustible source of reliable and environmentally benign energy on Earth. Despite the immense technical challenges involved in making magnetic fusion a source of commercial electrical power, important progress has been made in the past decade as researchers nationwide have collaborated on experiments and computer simulations.

Lawrence Livermore's Fusion Energy Program carries out magnetic fusion energy research in two complementary thrusts. The first thrust is performing advanced fusion experiments. Livermore researchers are collaborators at the national DIII-D tokamak experiment at General Atomics in San Diego, California.

Laboratory scientists are also pursuing novel designs for magnetic fusion reactors, such as the spheromak experiment dedicated in 1998. (See *S&TR*, December 1999, pp. 18–20.)

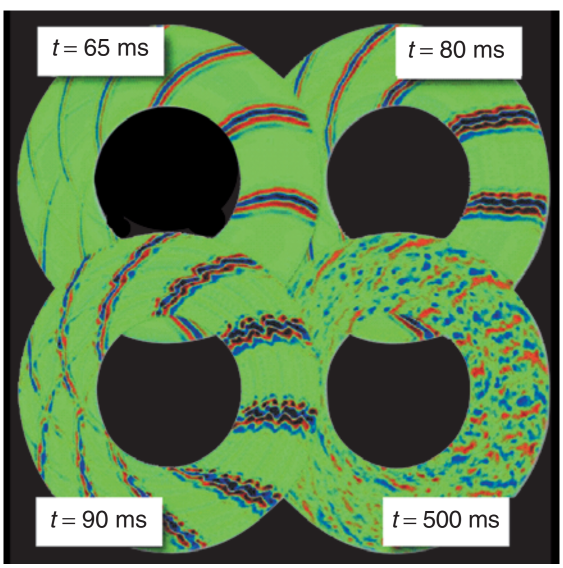
Complementing the experimental work is an effort to accurately simulate the extraordinarily complex physics involved in magnetically confined plasmas. Lawrence Livermore scientists have developed a number of codes for simulating different aspects of magnetic fusion energy experiments. Its PG3EQ program, developed by physicists Andris Dimits, Dan Shumaker, and Timothy Williams, for example, is one of the most advanced programs available for simulating plasma turbulence. Another Livermore code, called CORSICA, goes a step further and links individual programs that model different aspects of magnetic fusion energy physics. (See *S&TR*, May 1999, pp. 20–22.)

Focus on Tokamak

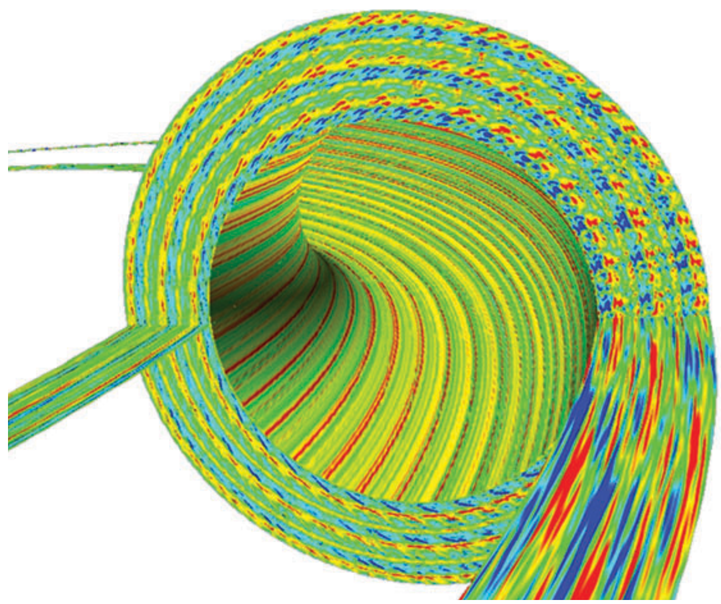
A national team of researchers led by Laboratory physicist Bill Nevins is developing advanced simulation codes running on supercomputers to deepen scientific understanding of the plasma turbulence that occurs inside a tokamak, a magnetic confinement device. Tokamaks use powerful magnets to confine plasmas of fusion fuel on the toroidal, or doughnut-shaped, magnetic “surfaces” defined by individual magnetic field lines as they wind about within a vacuum chamber.

Plasma turbulence causes thermal energy to leak across the magnetic surfaces faster than it can be replaced by fusion reactions. This lost energy must be replaced by external sources to prevent the plasma from cooling below the 100-million-degree temperatures needed to optimize the rate of fusion reactions. However, current tokamak experiments are close to the major goal of breakeven, that is, the point at which the energy produced by the fusion reactions equals the energy applied from an external source to heat the fuel. A better understanding of plasma turbulence may allow researchers to reduce the rate of energy loss so that energy breakeven could be achieved in the current generation of tokamaks.

The national collaboration is called the Computational Center for the Study of Plasma Microturbulence. It is funded by the Department of Energy’s Office of Fusion Energy Sciences, a part of DOE’s Office of Science. The work is part of the Office of Science’s Scientific Discovery through Advanced Computing (SciDAC) program, which was launched in late 2000. SciDAC’s goal is to develop the scientific computing hardware and software needed for terascale (trillion-operations-per-second) supercomputing. The effort is similar to the National Nuclear Security Administration’s Accelerated



This simulation, done by Livermore collaborator General Atomics of San Diego, California, with the GYRO code, shows a cross section of a tokamak over time (*t*) in microseconds (ms). The color contours indicate microturbulent fluctuations in the plasma density. The center sections have been removed to facilitate comparison.



Part of the cross section of a tokamak plasma. The color contours indicate microturbulent fluctuations in the plasma density. Livermore’s PG3EQ code, which was used to produce this simulation, models a “tube” of magnetic flux as it wraps once around the tokamak poloidally, or the short way around. Toroidal symmetry was then used to displace this flux tube and fill the annulus.

Strategic Computing Initiative, which is making available terascale computers for the nation's Stockpile Stewardship Program.

The collaboration involves researchers from Lawrence Livermore, the Princeton Plasma Physics Laboratory, the University of California at Los Angeles, the University of Colorado, the University of Maryland, and General Atomics. These institutions were part of previous DOE magnetic fusion energy simulation efforts, including the Numerical Tokamak Turbulence Project (1993 to 1999), led by Livermore physicist Bruce Cohen, and the Plasma Microturbulence Project (2000 to 2001), led by Nevins.

The simulations are focused on microturbulence, a long-time nemesis of achieving breakeven conditions in magnetic fusion energy experiments. Microturbulence is one of two forms of plasma turbulence observed in magnetic confinement experiments. Macroturbulence, on the scale of centimeters to meters, has been largely tamed in advanced tokamak designs. Microturbulence, on the scale of tenths of millimeters to centimeters, has not.

Fluctuating Plasma Soup

Microturbulence is an irregular fluctuation in the plasma "soup" of electrons and ions. The fluctuations are caused by gradients of density and temperature. The fluctuations, a collective phenomenon, form unstable waves and eddies that transport heat from the superhot core across numerous magnetic field lines out to the much cooler plasma surface and, ultimately, to the tokamak's walls. Energy researchers call this phenomenon energy transport.

Nevins notes that a tokamak's plasma will undergo fusion reactions only if it is hot enough, dense enough, and kept away from the much colder reactor walls. By causing heat to be lost from the plasma core, microturbulence helps to degrade confinement and prevent breakeven conditions. "We want plasma at about 100,000,000°C in the center and below 1,000°C at the walls, so they don't melt," says Nevins. "We obviously need good thermal insulation, and that's provided by the confining magnetic field. If we can minimize microturbulence, we can prevent heat leaking out faster than the fusion reactions can generate heat."

Controlling microturbulence will be immensely important in determining whether an advanced experiment, currently in the early planning stages, will be a success. Nevins says that the largest tokamaks cost several hundred million dollars to build. Constructing an experimental device that would go beyond breakeven for a net production of energy would cost about $2 billion. If a way were found to control microturbulence, construction costs could decrease significantly.

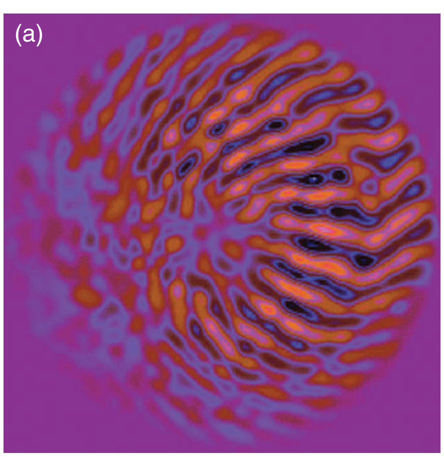
Says Cohen, "If we had better energy confinement, we could build the next generation device at a much lower cost. To do that, we need to understand better the nature of plasma microturbulence."

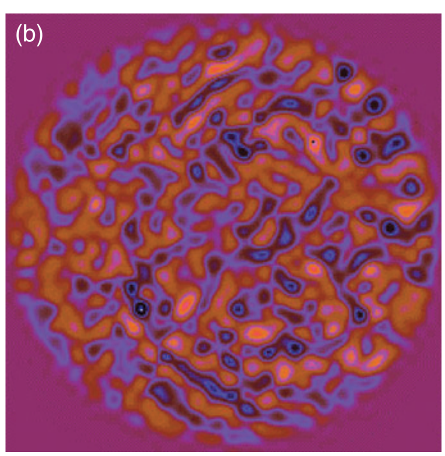
Simulation Focus

The collaboration's current focus is on advanced codes, algorithms, and data analysis and visualization tools. Nevins says that simulating microturbulence has proved difficult because of the enormous range of time and space scales that occur in magnetic fusion plasmas. Indeed, scientists within the national magnetic fusion energy program have worked to model microturbulence for more than two decades.

Fortunately, massively parallel computers, which use thousands of microprocessors in tandem, are well-suited to this simulation task. These machines are ideal because the collective behavior of trillions of electrons and ions is complex, but the underlying physics—and the equations that describe it—are relatively straightforward.

Most computing is done remotely at the





The UCAN code, developed by Livermore collaborators at the University of California at Los Angeles, produced these two images of tokamak plasmas. (a) Early in the development of the microturbulence, small-amplitude, radially elongated turbulent eddies form. (b) Fully developed microturbulence exhibits smaller, disordered structures.

Fusion for the Future

Fusion combines the nuclei of light elements to form a heavier element. For example, two nuclei of hydrogen isotopes, deuterium and tritium, will overcome the natural repulsive forces that exist between such nuclei and combine under enormous temperature and pressure. The fusion reaction produces a single nucleus of helium, a neutron, and a significant amount of energy.

A device that creates electricity from fusion must heat the fuel to a sufficiently high temperature and then confine it for a long enough time so that more energy is released than must be supplied to keep the reaction going. To release energy at a level required for electricity production, the fusion fuel must be heated to about 100,000,000°C, more than 6 times hotter than the interior of the Sun. At this temperature, the fuel becomes a plasma, an ionized gas of negatively charged electrons and positively charged ions. Although rare on Earth, plasmas constitute most of the visible universe.

The challenge for scientists is how to confine the plasma under extreme temperatures and pressures. One solution is to use powerful magnetic forces. In the absence of a magnetic field, a plasma's charged particles move in straight lines and random directions. Because nothing restricts their motion, the charged particles can strike the walls of a containing vessel, thereby cooling the plasma and inhibiting fusion reactions. In an appropriately designed magnetic field, the particles are forced to follow spiral paths about the magnetic field lines so they do not strike the vessel walls. The plasma is thus confined to a particular magnetic field line. The magnetic field line itself can be confined within a vacuum chamber if its path is restricted to a toroidal, or doughnut, shape.

A bundle of such magnetic field lines forms a doughnut-shaped magnetic "bottle" called a tokamak, an acronym derived from the Russian words meaning toroidal chamber and magnetic coil. In the tokamak, the stable magnetic bottle is generated both by a series of external coils, which are wrapped around the outside of the doughnut, and by a strong electrical current, up to several million amperes, that is induced in the plasma itself.

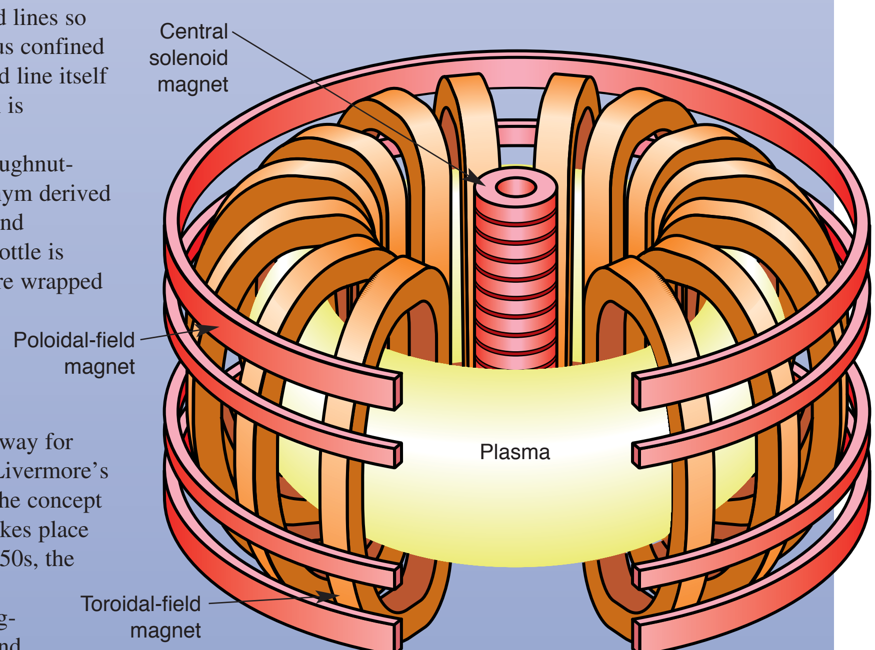
Half Century of Research

Magnetic fusion energy research has been under way for more than a half century and was one of Lawrence Livermore's original programs. The idea was classified because the concept uses the energy released by the same reaction that takes place in a hydrogen or thermonuclear bomb. In the late 1950s, the research program, called Project Sherwood, was partially declassified because it was viewed as a long-term effort without immediate military application and one that would benefit greatly from international cooperation.

Considerable progress has been made in the last 20 years at Livermore and other research centers in meeting the scientific challenges of attaining the combination of temperature, density, and confinement time necessary to promote fusion reactions. At one point, several different types of devices, including Livermore's magnetic "mirror" design, were pursued within the national program. Budget constraints, however, led to the adoption of the tokamak as the principal design for the U.S. program, with other approaches being explored at lower levels of resources.

The long-standing goal of magnetic fusion energy is to produce abundant, environmentally acceptable electric energy from a fusion-powered reactor. In fusion power plants, the heat from deuterium–tritium fusion reactions would be used to produce steam for generating electricity. Deuterium is abundant and easily extracted from ordinary water (about one water molecule out of every 6,000 contains deuterium). Tritium can be made from lithium, a plentiful element in Earth's crust.

One kilogram of deuterium–tritium fusion fuel would produce the same energy as 30 million kilograms of coal. Other major advantages include no chemical combustion products and therefore no contribution to acid rain or global warming, radiological hazards that are thousands of times less than those from fission, and an estimated cost of electricity comparable to that of other long-term energy options.



In a tokamak, magnetic fields from surrounding magnets confine a plasma fuel of hot, ionized gas within a hollow, doughnut-shaped vacuum chamber.

Department of Energy's National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory. In fact, the collaboration is the biggest user of NERSC facilities. The current simulations typically require from 10 to 20 hours to complete using NERSC's most powerful machines.

With the latest generation of supercomputers, says Cohen, "We can do bigger pieces of the simulation, with more physics." Nevertheless, no computer yet built can perform simulations requiring six orders of magnitude in spatial size, eight to nine orders of magnitude in time scale, and three dimensions in space. As a result, "We have to be clever about reducing the scales and still obtaining accurate results," says Cohen.

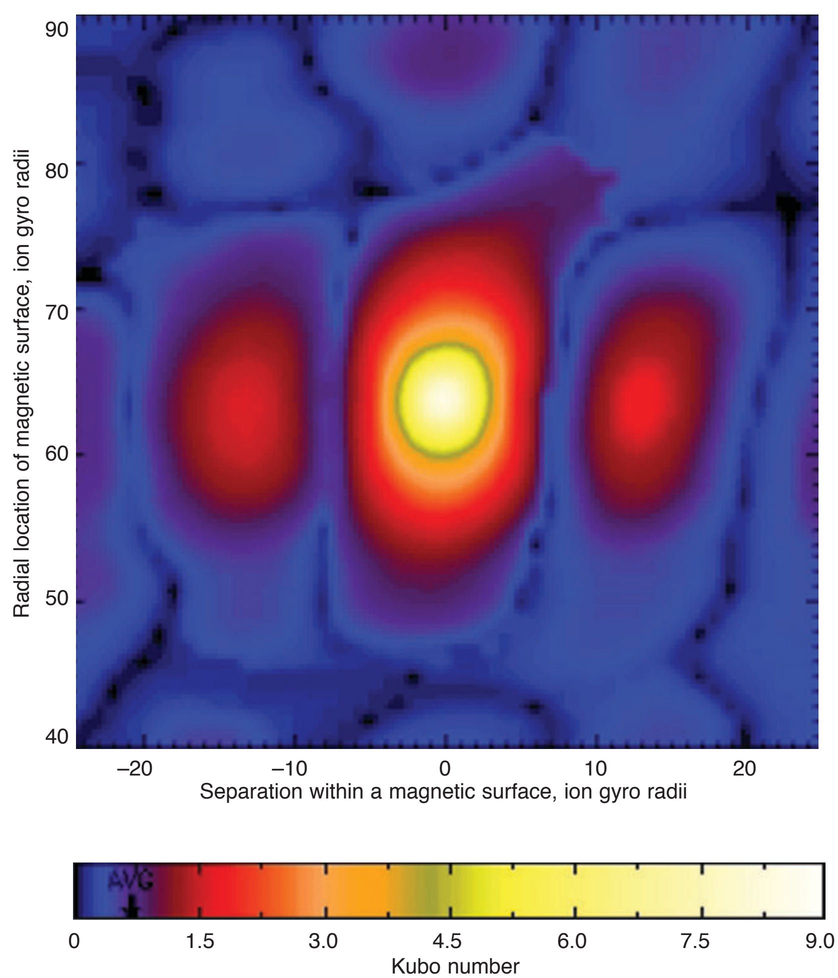
The hardware advances have been accompanied by the equally impressive development of efficient algorithms with which to solve the equations that form the basis of plasma simulation. The algorithms are of two kinds, particle-in-cell (PIC) models and continuum models, depending on how they track simulated electrons and ions in space and time. PIC models track individual electrons and ions; continuum models solve equations that do not involve individual particles.

The national effort is developing both kinds of algorithms because they offer a valuable means of verifying new codes. "Together, the two kinds of algorithms provide a balanced scientific approach to understanding microturbulence," says Nevins. Each approach, however, pushes the limits of current supercomputer capability.

PIC and continuum algorithms can be used in two geometric representations: global and flux tube. Global simulations model the entire plasma core of a tokamak, whereas flux tube simulations represent a more limited area. Here again, says Nevins, the two geometric approaches serve as a useful cross-check on the results obtained from each other.

With the increased speed of microprocessors, additional memory, massively parallel supercomputers, and advanced algorithms, important progress has been made in the past few years in modeling microturbulence. Nevins points to significant improvements in the comparisons of simulations to experiment results, in the agreement of results from codes developed by collaborators from different centers of magnetic fusion energy research, and in the increasingly thorough and accurate physics content of the models.

An important aspect of the code work is developing new tools to analyze and visualize the simulation results. Data analysis and visualization provide the bridge between the microturbulence simulation and experimental research. Nevins has developed GKV, a program that allows the user to easily compute, analyze, and display results (in presentation-quality



Livermore's GKV program allows users to interactively compute, analyze, and display data from microturbulence simulations. This GKV image displays the Kubo number, or the number of times an ion circulates around a turbulent eddy before that eddy dissipates, versus the separation within a magnetic surface and the radial location of the magnetic surface. Distances are measured in ion gyro radii, that is, the radius of a typical ion's orbit as it gyrates about a magnetic field line.

form) easily from microturbulence simulation data. The program is used by researchers nationwide.

A strong numerical model of microturbulence, combined with better data analysis and visualization tools, is aiding the interpretation of experimental data and the testing of theoretical ideas about microturbulence and how to control it. The simulations are also helping scientists to plan future experiments. In addition, continued progress in code development may stimulate advances in the understanding of astrophysical plasmas and turbulence in fluids.

Theorists Now Getting Respect

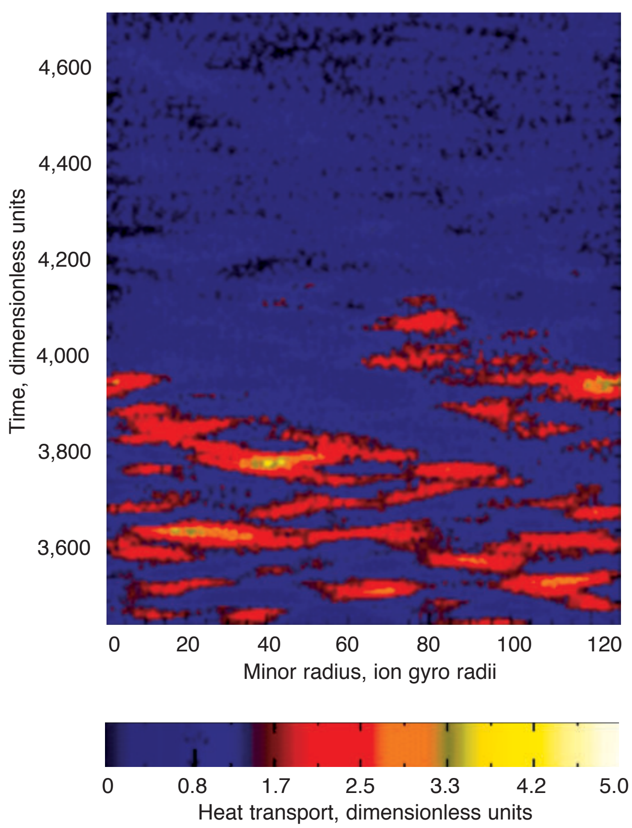
Cohen recalls that five years ago, experimentalists paid much less attention to theorists regarding plasma turbulence. Today, however, simulations do such a good job in predicting experimental results that "experimentalists are really paying attention to the codes." Simulations, he says, have achieved such a level of fidelity to the underlying plasma physics that they can often be used as a tool for experiments regarding plasma microturbulence.

Nevins points out that the cost of doing simulations is nearly negligible compared with the cost of building and running a new fusion ignition experiment (around $1 billion to $2 billion). "Inexpensive but increasingly realistic simulation capability will continue to have immense leverage on relatively expensive experiments," he says.

He also points out that numerical simulation has a distinct advantage over experimental observations of microturbulence: The simulations give users access to virtually any portion of the plasma in time or space. Simulations use "synthetic" diagnostic tools, which mimic the signal that an experiment would be expected to produce on an experimental diagnostic.

Says Nevins, "We can put in better diagnostics on a computer code than we can during an experiment." What's more, the physics underlying observed microturbulence can often be ambiguous. "With a simulation, we can turn different physics on and off to isolate what is driving the microturbulence observed in the experiment."

Not only have recent simulations produced a clearer understanding of microturbulence, but they have also provided a few surprises as well. For example, scientists have long puzzled over large but transient bursts of heat that are transported out of the core plasma by microturbulence eddies. "We would have expected the transfer of heat from the plasma core out to the walls to be homogeneous because of the small eddies caused by microturbulence. Instead, we've seen large, intermittent bursts 10 times the size of the eddies," Nevins says.



Tokamak experiments have detected puzzling bursts of heat produced by microturbulence. Recent simulations show the same phenomenon, where the heat pulses are indicated by bright regions. Researchers have noticed the similarity between these heat pulses and other instances of self-organized criticality, which resemble the sudden occurrence of avalanches as grains of sand are slowly added to the top of a sandpile. The simulation also shows the spontaneous transition in time from a state of high heat transport, with many heat pulses, to a state of low heat transport, in which the heat pulses are largely absent. This transition was caused by microturbulence-induced changes in the plasma's flow shear.

Learning from Sandpiles

Nevins and others have noticed that these intermittent spikes are characteristic of "self-organized criticality," a phenomenon that occurs in a system when certain key parameters reach critical values. Self-organized criticality is responsible, for example, for the occurrence of sudden avalanches as grains of sand are slowly added to the top of a sandpile. The Livermore simulation team is using the insights derived from self-organized criticality to account for these unexpected bursts of heat, which apparently are the combination of many turbulent eddies.

An important recent addition to the simulation codes is a phenomenon called flow shear that works to dampen microturbulence and thereby improve plasma confinement. The plasma rotates (flows) within each of the nested magnetic surfaces defined by individual magnetic field lines. The term flow shear describes spatially localized changes in the rate of plasma rotation. The flow shear sharply reduces the rate at which heat is transported out to the cold plasma edge by stretching and tearing apart the microturbulence eddies.

Nevins explains that heat must travel to the outer plasma edge across many nested magnetic surfaces. When the magnetic surfaces rotate relative to each other, the eddies transporting the heat tend to dissipate. He offers the analogy of a busy freeway, with each lane of cars (magnetic surface) at a different speed. If a driver must hand a rubber band (microturbulence eddy) to a driver in another lane passing by at a much faster rate, the rubber band will soon break and not be passed to the driver in the faster lane.

Flow shear can appear spontaneously during a magnetic fusion energy experiment. When that happens, says Cohen, “We get it for free.” Flow shear can also be created experimentally by applying a twisting force (torque) to the plasma using, for example, intense beams of neutral hydrogen atoms. The force pushes on the center of the plasma core to create barriers to heat transport.

“We want to understand much better how flow shear functions so we can know how much to apply to effectively control microturbulence,” says Cohen. Precisely applying flow shear could increase plasma confinement and significantly decrease the cost of new experimental facilities.

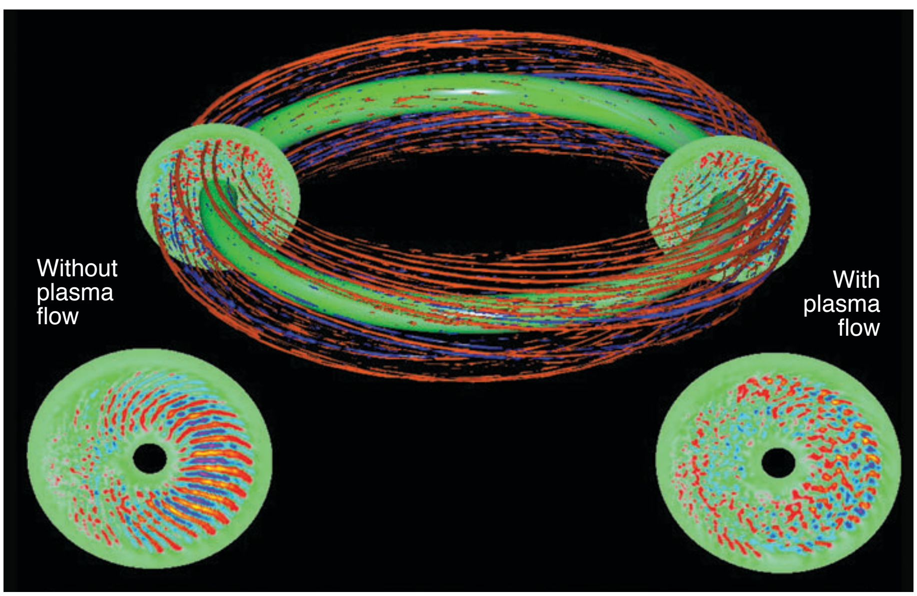
The national collaboration is working to provide a suite of modular, complementary computer programs, each with an identical user interface. Together, the modules will constitute a comprehensive code for microturbulence simulation, data analysis, and visualization. The modular architecture will enable physics simulations on diverse computer architectures with much less effort than current software approaches demand. Says Nevins, “We want to revolutionize the fusion community’s ability to interpret experimental data and test theoretical ideas. The result will be a much deeper understanding of microturbulence.”

As for the codes themselves, the collaborators are working on consolidating programs developed by individual research groups. Another area of activity is improving the physics simulated by the codes, for example, by refining the simulated diagnostic instruments and more accurately modeling the role of electrons involved in microturbulence.

Nevins is hopeful that by making the simulations easier to run and analyze, even more experimenters will choose to use them. “It was a heroic feat to make the codes work, but now we need to make them available to the experimental community,” he says. “We want these tools to be used more widely so that we expand the use of microturbulence simulation well beyond the existing small group of code developers. Our goal is to have experimentalists run the codes and understand the results much faster.”

Better simulation tools could bring dependable fusion energy much closer to reality. That would be welcome news for a nation recently reminded about the fragility of steady energy supplies and prices.

—Arnie Heller



Simulation of a tokamak and two plasma cross sections. In the simulation that produced the plasma cross section on the left, the flow shear was suppressed, while the self-generated flow shear was retained in the simulation that produced the cross section on the right. These cross sections illustrate the role of flow shear in suppressing plasma microturbulence and thereby forming barriers to unwanted heat transport. This simulation was created using the GTC code developed at the Princeton Plasma Physics Laboratory.

Key Words: fusion, macroturbulence, magnetic fusion, microturbulence, National Energy Research Scientific Computing Center (NERSC), plasma, Scientific Discovery through Advanced Computing (SciDAC), tokamak, turbulence.

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From Kilobytes to Petabytes in 50 Years

"The day when the scientist, no matter how devoted, can make significant progress alone and without material help is past."
—E. O. Lawrence, founder of Lawrence Livermore National Laboratory, on accepting the 1939 Nobel Prize for Physics

THE history of Lawrence Livermore National Laboratory is inexorably tied to the evolution of supercomputers—the largest, fastest, most powerful computers in the world. Even before the Laboratory's gates opened for the first time in September 1952, founders E. O. Lawrence and Edward Teller recognized that computers were needed to better calculate the thermonuclear explosions for the nuclear weapons the "Rad Lab" in Livermore was destined to design.

Designing nuclear weapons and predicting their behavior has always been a difficult technical and scientific challenge. In a thermonuclear explosion, matter is accelerated to millions of kilometers per hour while experiencing densities and temperatures found only in stars. In addition, weapon designers needed to identify and understand the important physical properties of matter under these exotic conditions. With little experimental data available, Livermore's designers turned to computers to simulate and visualize the processes and the physics of nuclear weapons.

To fulfill its critical national defense mission, the Laboratory constantly sought out the most advanced computers with the most capability. In the 1990s, with the cessation of underground nuclear testing, advanced supercomputers figured prominently in plans for stockpile stewardship, helping scientists predict the behavior of the aging nuclear stockpile to better assess its safety, reliability, and security.

Mag Tape and Punch Cards

Livermore's first supercomputer, the Remington-Rand Univac-1, had 5,600 vacuum tubes and was over 2 meters wide and 4 meters long. Between April 1953 and February 1957, the Univac executed as many calculations as 440 human "calculators" could perform in 100 years if they worked 40 hours a week, 52 weeks a year, and made no mistakes. Memory, however, was an issue.

The Univac's memory consisted of mercury tanks that could store 9 kilobytes of data—a tiny fraction of what today's pocket-sized handhelds can hold. The code that performed all its operations was stored on magnetic tapes that had to be loaded into the machine in parts. Calculations could involve as many as nine tapes, and the nine reel mechanisms were troublesome, accounting for much of the machine's 25 percent downtime. Clearly, machines with more memory were needed.

With the arrival of the IBM 701 in 1954, scientists expected that nuclear explosives computations would run much faster. The IBM, which was the first fully electronic computer, was 12 times faster than the Univac, had twice the memory, and primarily used punch cards for input and output. Scientists took advantage of the improved capabilities to increase resolution and add more detailed physics, so the computational runs continued to average 100 hours.

A series of IBM machines followed the 701. The IBM 704—twice as fast as the 701—even played a part in the early

Weapons

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space race between the U.S. and the Soviet Union. Soon after the launch of the Soviet Sputnik I satellite in October 1957, the Laboratory received an urgent request to help predict when the satellite would come back to Earth. Livermore's IBM 704s were the only computers in the U.S. able to perform the calculations. Joe Brady, a now-retired Laboratory scientist, recalls, "We used two 704s for 70 hours straight, only stopping to rush outside to see the satellite orbiting overhead." Laboratory computation workers accurately calculated the satellite's plunge into the atmosphere in early December, an extrapolation of 58 days from launch. The 704s eventually gave way to IBM 709s, which were faster still, thanks to special-purpose input/output channels to speed up processing, and batch processing—a new technique that permitted many individual tasks to be processed without a human operator's assistance.

In the late 1950s, Edward Teller proposed that the Laboratory commission a computer from commercial suppliers. In May 1960, Remington-Rand delivered the Livermore Advanced Research Computer (LARC) built to Livermore's specifications. At that time, there was an international moratorium on nuclear testing, and upgraded computing capabilities were urgently needed by weapon designers. With a high-speed magnetic core memory for storing about 240 kilobytes and 12 auxiliary memory drums for storing about 24 megabytes more, the LARC had such dense wiring that technicians had to use special tools similar to surgical instruments to probe its insides. Next came the "Stretch," an IBM machine with about 780 kilobytes of memory that could perform 100 billion calculations in a day.

As the 1960s progressed, the computer market changed. Most manufacturers abandoned the highly specialized large-computer market of the national laboratories to concentrate on the computer needs of the rapidly growing business and financial markets. In 1963, the Laboratory turned to Control Data Company (CDC), which furnished all of Livermore's supercomputers for the next 15 years, including the CDC 6600 in 1964 and the CDC 7600—10,000 times faster than the original Univac-1—in 1969. The Laboratory received serial number 1 of each of the machines and, by using them, helped CDC ready their computers for the wider commercial market.

The Univac was the first computer to store information on magnetic tape. Running a program was a hands-on operation, with a physicist or programmer toggling console switches to execute the problem. Although highly accurate, the Univac was cantankerous, breaking down two or three times a day. Early workers regarded it as an "oversized toaster."

Entering a Parallel Universe

About this time, computers began exploiting computational parallelism. The CDC STAR-100s in 1976, followed by the Cray 1s, introduced vector architectures. Cray came out with the first closely coupled processor systems with its two-processor Cray X-MPs. The final Cray machine, installed at the National Energy Research Scientific Computing Center (now located at Lawrence Berkeley National Laboratory), had 16 central processing units (CPUs) and about 2 megabytes of memory.

In the early 1990s, massively parallel machines—that is, employing scalar architectures—such as the Meiko and the BBN (by Bolt, Beranek, and Newman) began to arrive at the Laboratory. As Mike McCoy, a deputy associate director for Livermore's Computation Directorate, explains, "About this time, we began looking at not just sheer capability, which has been the motivator at the Lab since day one, but price performance as well. Up to and including the Crays, we would depend on a single vendor to supply the capability we needed.

Part of getting the price performance we needed involved moving away from specialized processors for parallel machines to commodity processor systems.” The Meiko and the BBN were the first supercomputers of this type. Instead of using a few, enormous, one-of-a-kind processors, the Meiko and the BBN used many mid-sized workstation processors (the BBN, for instance, had 128 such processors). “We learned how to build software for parallel systems on these computers,” notes McCoy. “These systems were what made us able to transition to the massively parallel ASCI [Advanced Simulation and Computing program, formerly called Accelerated Strategic Computing Initiative] systems.”

In 1995, the Department of Energy and its defense laboratories—Livermore, Los Alamos, and Sandia—were directed to undertake the activities necessary to ensure continued stockpile performance in the absence of underground nuclear testing. DOE’s ASCI program is a key component to meeting this challenge. The ASCI program is developing a series of ever more powerful, massively parallel supercomputers that employ thousands of processors working in unison to simulate the performance of weapons in an aging nuclear stockpile. The second ASCI supercomputer—the Blue Pacific, built by IBM—was received at Livermore in September 1996. It was installed, powered up, and running calculations within two weeks. IBM’s ASCI White, which was delivered to the Laboratory in three stages during the summer of 2000, is currently the world’s most powerful computer. Performing 12 trillion operations per second (teraops), it is 30 billion times faster than the Laboratory’s very first computer, the Univac-1.

In late 1999, Livermore researchers achieved a major milestone with the first-ever three-dimensional simulation of a nuclear weapon’s primary (the first stage of a hydrogen bomb) using the ASCI Blue Pacific. The simulation ran a total of 492 hours on 1,000 processors and used 640,000 megabytes of memory in producing 6 million megabytes of data contained in 50,000 graphics files. A second major milestone, a three-dimensional simulation of a nuclear weapon secondary, was completed on ASCI White in spring of 2001. Late in 2001, Livermore and Los Alamos met a third milestone on this system, coupling the primary and secondary.

Forward to the Future

With all that has occurred in the last 50 years, it’s nearly impossible to predict what the far future will hold. “To meet ASCI’s requirements, more powerful processors with more memory are needed to create a proxy of the world around us, from the microscale to the macroscale,” says Dona Crawford, associate director of Computation. “At the same time, we are creating terabytes—soon to be petabytes—of data.” Two trends, Crawford notes, need to continue into the near future. First, the Laboratory must acquire faster processors with more memory for simulation and modeling. Second, new ways must be created for storing, finding, visualizing, and extracting the data. “We need to merge high-end computing and high-end information technology,” she concludes. “Scientific data management, in particular, is becoming more of an issue.” (See the box on software development, p. 23.)

Within three years, the ASCI community plans to locate a 60-teraops machine with approximately 20,000 processors—the Purple machine—at Livermore in the soon-to-be-built Terascale Simulation Facility. Groundbreaking for this facility will occur in spring of this year. Beyond Purple lies a world of tantalizing prospects, including BlueGene/L (L stands for

The ASCI White, with power to perform 12 trillion operations per second, was delivered to the Laboratory during the summer of 2000.

Software Development

The supercomputers Livermore acquired were often the first of their kind—sometimes even prototypes of the final version—and had little support software. As a result, Livermore's scientists took the lead in developing software for operating the system (such as assemblers, loaders, and input/output routines) as well as for simulating and modeling physical phenomena. Because Laboratory users pushed the machines to their limits, Livermore's programmers had to find—or often invent—the most efficient programming and computing techniques. For instance, when certain aspects of the FORTRAN computer language turned out to be awkward or limiting for scientific applications, software developers created an enhanced version called LRLTRAN (Lawrence Radiation Laboratory FORTRAN). It took nearly two decades for many of the advanced features in LRLTRAN to be incorporated into standard FORTRAN. In addition, Livermore developed the time-sharing concept—in which a central processing unit (CPU) alternates between working on several jobs at once rather than one at a time—into its first practical use for supercomputers. The Laboratory also led the way in computational physics (the numerical simulation of physical phenomena) on supercomputers. Computer codes often hundreds of thousands of lines long are used to model complex processes that are too difficult or impossible to calculate exactly.

This expertise in codes continues today, with computer scientists writing or adapting codes for large parallel machines such as the Advanced Simulation and Computing (ASCI, for its former name, Accelerated Strategic Computing Initiative) systems. The sophisticated codes now under development promise a level of physical and numerical accuracy more like that of a scientific experiment than a traditional numerical simulation. In materials modeling, for instance, ASCI White will track 10 billion atoms simultaneously, beginning to predict what scientists will see when imaging materials through electron microscopes.

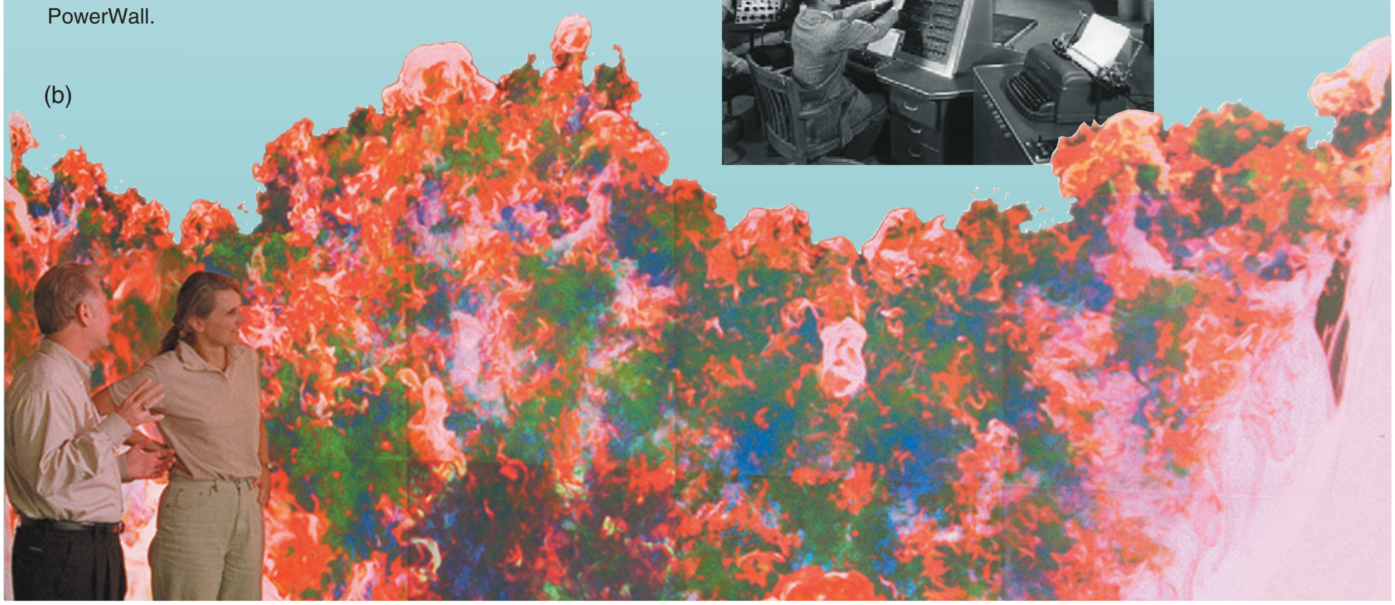
Interpreting, visualizing, and accessing the data are themselves challenges. From the early days of simple x–y plots to today's complex three-dimensional images, Livermore computer scientists have developed programs to help researchers access massive quantities of data in visual formats. This capability is particularly important for the future, given that ASCI-level supercomputers generate terabytes—soon to be petabytes—of raw data.

As computers grow in speed, number-crunching capability, and memory, scientific researchers edge into data overload as they try to find meaningful ways to interpret data sets holding more information than the U.S. Library of Congress. Livermore's computer scientists are exploring techniques such as metadata, data-mining, and visualization to deal with the massive amounts of data.

(a) Results from Univac computations were spewed out as reams of numbers by a Remington-Rand typewriter modified to serve as an on-line printer. (b) Results from today's complex simulations are converted by powerful visualization software into three-dimensional detailed views, such as this one shown on the Livermore-developed PowerWall.

(a)

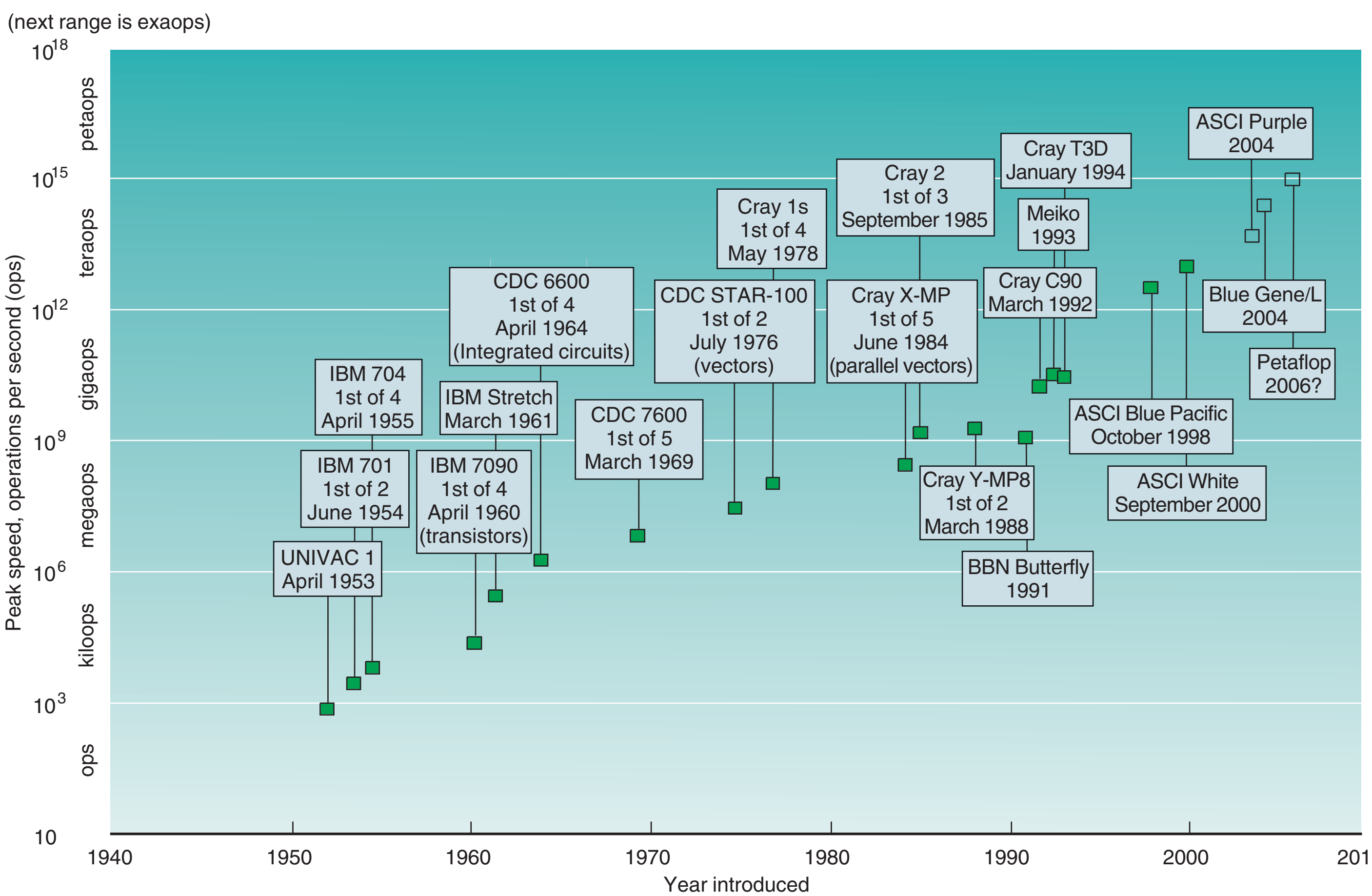
(b)



light), a machine 15 times faster than today's fastest supercomputers. "BlueGene/L would be a radical departure from previous machines," notes Mark Seager, program manager for ASCI Terascale Systems. BlueGene/L would use IBM's "system on a chip" based on commercial embedded-processor technology. Seager explains, "Embedded processors are optimized for low cost and low power and for usability in many configurations." McCoy notes that systems like BlueGene/L are the next big step in getting more performance at a lower price. "From ASCI Red to Purple, the systems use workstation processors targeted at the high-performance computing market. With BlueGene/L, we'd move from that curve to one using commodity PC processors. At the same time, we'd also move from using proprietary vendor software to open-source software such as the Linux operating system. These moves would result in considerably lower costs for the power we'd get—about $0.1 million per teraops for BlueGene/L, compare with White's $9 million per teraops or Purple's $3 million per teraops."

BlueGene/L would have 65,000 nodes or cells, 360 teraops—larger than the total computing power of the top 500 supercomputers in the world today—and between 16 and 32 terabytes of memory. "The questions facing us for BlueGene/L are: Can we build it? Can we write software for it? Can we write scientific simulations for it? We believe the answers are 'yes' to all," says Seager. Six times more powerful than ASCI Purple, BlueGene/L would open new

A rendering of the Terascale Simulation Facility, which will house ASCI Purple, a machine capable of performing 60 trillion operations per second.



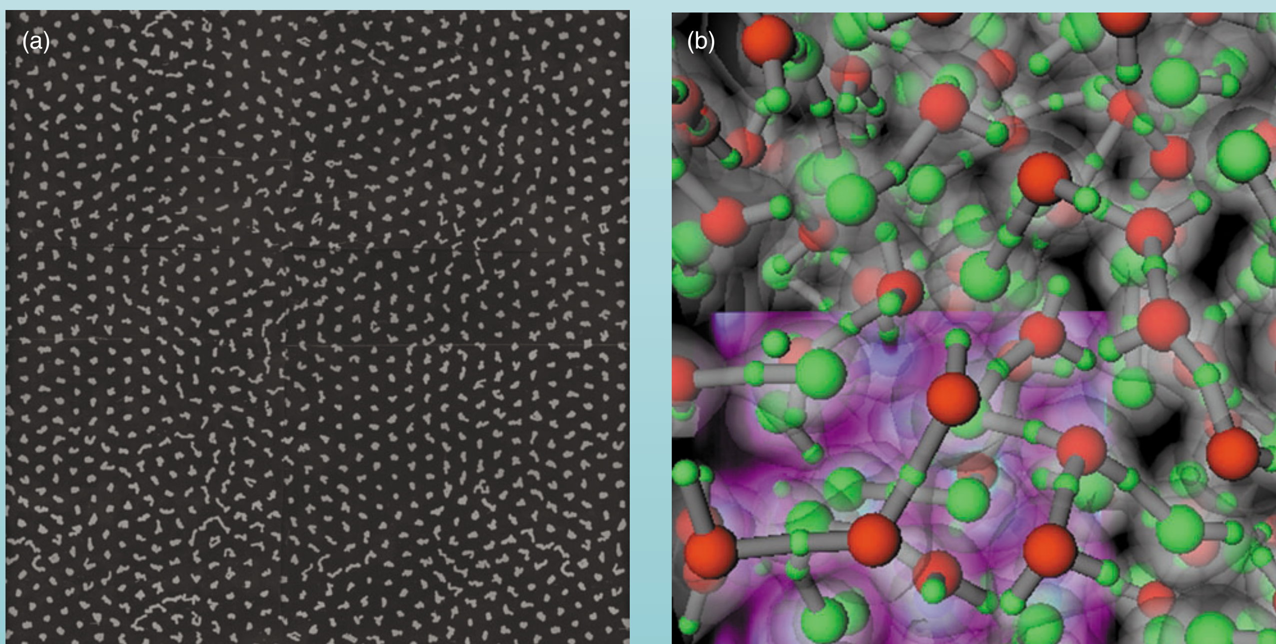
Timeline of Livermore's key supercomputers and their peak computing power.

From Personal Computers to Clusters

While supercomputers were always an integral part of Livermore's nuclear weapons design and stockpile stewardship efforts, other areas of the Laboratory also benefited from the computer revolution, particularly as computer systems became smaller, more powerful, and less expensive. In the 1970s, small microprocessor systems such as the PDP-11 began to be used in research tasks—digitizing oscilloscope traces, for example, and controlling experiments in chemistry labs. Then the personal computer, or PC, arrived, followed by more powerful microcomputers and workstations.

By the mid-1990s, many researchers in nonweapons areas were taking advantage of the relatively inexpensive and powerful desktop computers in their offices, or they used terminals tied to scientific workstations. Although having many advantages, these machines did not always have the necessary computational power, particularly for running three-dimensional simulations, which require the enormous computational horsepower of the latest generation of supercomputers. Finally, in 1996, Livermore programs and researchers outside the stockpile stewardship effort gained access to unclassified Accelerated Strategic Computing Initiative–level terascale supercomputers through the Multiprogrammatic and Institutional Computing Initiative (M&IC). (See *S&TR*, October 2001, pp. 4–12.)

The M&IC acquired increasingly more powerful clusters, or groups, of computers such as the Compaq TeraCluster2000. As the Laboratory begins to celebrate its 50th year, Livermore researchers are at the forefront of simulating a wide range of physical phenomena in the unclassified arena, including the fundamental properties of materials, complex environmental processes, biological systems, and the evolution of stars and galaxies. Mike McCoy, deputy associate director for Integrated Computing and Communications, says, "Livermore Computing has become an institutional resource much like the library, a place where researchers from any program can expect resources to support their research."



Particle tracking past and present contributes to a better understanding of the fundamental properties of materials. (a) In this example of Livermore physicist Berni Alder's pioneering computer simulation work, published in *Physics Review* in 1962, a simulation performed on the Livermore Advanced Research Computer supercomputer tracked 870 particles over time. (b) Recent work on the ASCI Blue Pacific includes this quantum-level simulation of a mixture of hydrogen fluoride and water molecules at high temperatures and pressures. The simulation tracked hundreds of atoms and thousands of electrons extremely accurately.

vistas in scientific simulation. “For instance,” says Seager, “you begin to approach what you need to model complex biological systems. Having BlueGene/L would be like having an electron microscope when everyone else has optical microscopes, it’s that much of a leap forward.”

And after that? “Perhaps there will be computers that align DNA to do processing, or Josephson junction machines, or all-optical machines. Who knows what will happen in hardware, software, and information technology in the next 50 years,” says Crawford. “Whatever innovation ends up driving the next era in computing will probably explode on the scene, much like the Internet did.”

Fifty years ago, the birth of the electronic scientific computer ushered in a new era. Rather than having to accept crude approximations because the more exact equations were too difficult to solve, scientists could use the great speed and high accuracy of computers to simulate the phenomena they were trying to understand. Livermore researchers pushed the limits of each advanced machine, from using crude one-dimensional codes on the Univac and early IBM machines to complex three-dimensional codes on the current ASCI machines. Through ASCI and the coming generations of supercomputing machines, another era appears on the horizon, an era in which enormously fast and powerful supercomputers will allow computer simulation to come into its own as a predictive science along with theory and experiment.

—Ann Parker

Key Words: Advanced Simulation and Computing (ASCI), ASCI BlueGene/L, ASCI Purple, ASCI White, computation history, Cray, IBM, Livermore Advanced Research Computer (LARC), supercomputer, Univac.

For further information, see the following Web sites on computation, past and present:

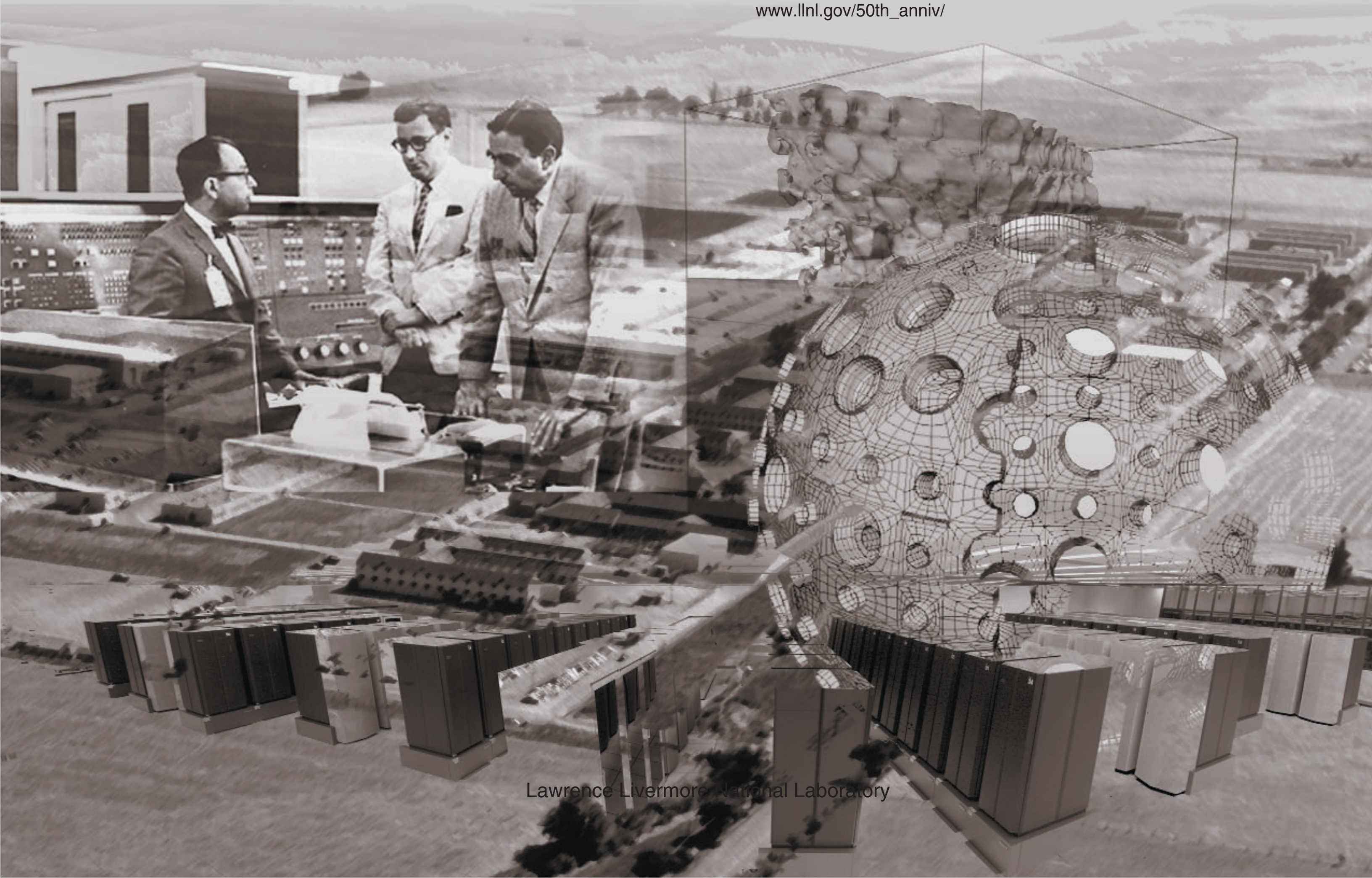
Computation at LLNL:
www.llnl.gov/comp/

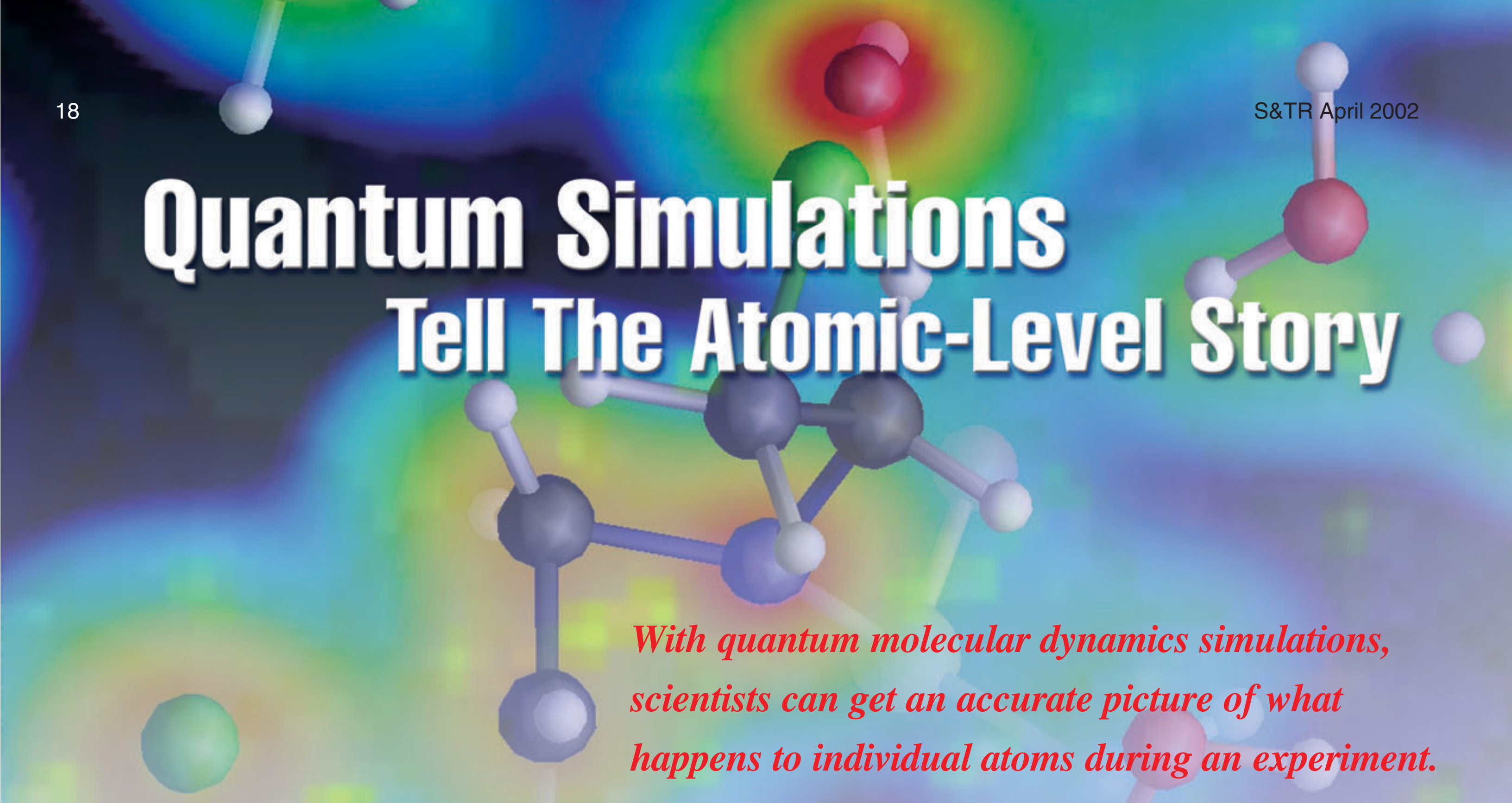
ASCI at LLNL:
www.llnl.gov/asci/

Oral History of Computation at LLNL:
www.nersc.gov/~deboni/Computer.history/

For further information about the Laboratory’s 50th anniversary celebrations, see the following Web site:

www.llnl.gov/50th_anniv/





Quantum Simulations Tell The Atomic-Level Story

With quantum molecular dynamics simulations, scientists can get an accurate picture of what happens to individual atoms during an experiment.

FOR almost as long as Lawrence Livermore has existed, scientists have been experimenting with materials to learn what happens to them under high pressure. In the brief instant of a high-explosive detonation, for example, shock waves produce pressure up to 500,000 times that of Earth's atmosphere, detonation waves travel as fast as 10 kilometers per second, and temperatures soar to 5,500 kelvins.

Early high-pressure experiments were designed to investigate the properties of weapon materials under these mind-boggling conditions and thus support the development of new weapons. Today, experiments seek out the fundamental properties of such deceptively simple materials as water and hydrogen. This very basic information is being applied to work in high explosives, planetary science, and materials science.

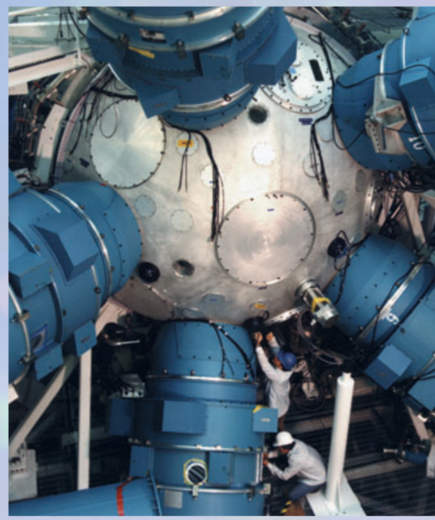
Experiments with a gas gun that shocks a sample or with a diamond anvil cell that applies static pressure demonstrate the changes brought about by pressure—the "after" conditions that scientists can compare to the "before." Now, for the first time, using computer simulations, researchers can get an accurate look at what happens to individual atoms and molecules during those experiments.

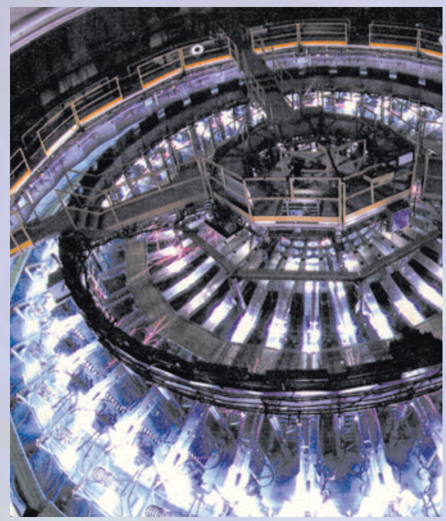
Simulations based on quantum molecular dynamics make it possible to view experimental activity as it happens. Quantum molecular dynamics is quite different from classical molecular dynamics, which is primarily concerned with the classical motion of atoms interacting with a given potential. The interesting chemistry and physics of many molecules take place at the atomic and subatomic level. But Newton's laws of classical mechanics no longer apply here. Physicists developed quantum mechanics early in the 20th century to appropriately describe the physics and chemistry of matter at the microscopic level. Quantum molecular dynamics focuses on all the interactions between atoms and electrons and does not involve fitting interactions to experimental data.

First-principles, or ab initio, molecular dynamics models use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. (See the box on p. 8.) These models in combination with Livermore's powerful computers allow scientists to create accurate, reliable simulations of complex physical phenomena.

Physicist Giulia Galli leads the Quantum Simulations Group at Livermore. In the four years since this group was established, it has explored entirely new territory. Early work included simulations of the mixing of water and hydrogen fluoride, DNA, and the elasticity of silicon carbide, a semiconductor material. (See *S&TR*, July/August 1999, pp. 20–22.) Their more recent simulations of shocked liquid hydrogen were the largest ab initio simulations to date on Livermore's terascale computers, which are part of the National Nuclear Security Administration's Advanced Simulation and Computing (ASCI) program. "Our hydrogen simulations were the first to look at an experiment in action," says Galli. "We could actually see how a real experiment had gotten from 'before' to 'after.'"

Quantum simulations are an excellent tool for predicting the properties of materials that cannot be measured directly. They provide accurate information about the properties of materials subjected to extreme conditions (for example, high temperature or high pressure) that are difficult to achieve experimentally. Simulations also help experimental physicists to interpret their results. "Simulation results neatly complement experimental results and may also guide the choice of new experiments," says Galli.





Experiments on (left) Livermore's Nova laser and (right) Sandia National Laboratories' *Z* accelerator shocked liquid deuterium, an isotope of hydrogen. In both experiments, a short, intense shock caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. The experiments found different compressibilities, which could affect the equation of state for hydrogen and its isotopes. Quantum simulations sought to point out physical reasons for the differences.

Codes Make It Work

The computer code used to simulate dynamic processes is JEEP, which physicist Francois Gygi began developing about eight years ago when he was at the Swiss Federal Institute of Technology. Some physical properties of matter, such as optical properties, can be obtained more accurately using static calculations performed with quantum Monte Carlo codes, which are the specialty of physicists Andrew Williamson, Jeff Grossman, and Randy Hood.

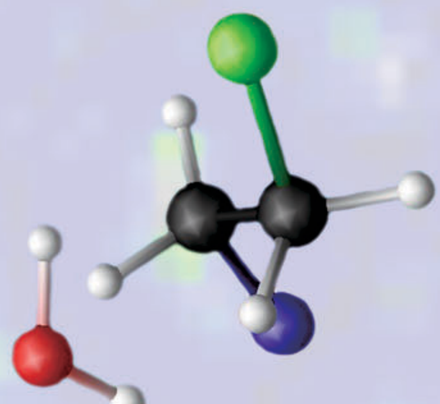
JEEP and quantum Monte Carlo codes operate differently. Both have to make approximations in their equations, but quantum Monte Carlo codes make very few. JEEP operates faster and excels at deriving the location of atoms and molecules. The more accurate quantum Monte Carlo simulations cannot give dynamic properties but are a better tool for determining the optical properties of molecules. Quantum Monte Carlo calculations are also useful for testing the validity of approximations made in the JEEP code's theory and for improving the accuracy of this theory.

Simulations Resolve Differences

Quantum simulations by Galli and Gygi may point out the differences found during two sets of high-pressure experiments on deuterium, an isotope of hydrogen with one proton and one neutron. One set of experiments was performed on Lawrence Livermore's Nova laser. The other set was performed on Sandia National Laboratories' *Z* accelerator, the world's most energetic pulsed-power machine, in Albuquerque, New Mexico.

The Livermore experiments in 1997 and 1998 and the Sandia experiment in 2001 subjected a sample of liquid deuterium to a short, intense shock that caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. In the Nova experiments, a laser beam produced a steady shock wave aimed at the target cell holding the sample. The wave was smoothed to ensure a spatially planar and uniform shock front, critical for obtaining accurate measurements.

The experiment at Sandia used an entirely different technique for producing a shock wave. Pulsed-power machines have large banks of capacitors used to accumulate electrical charges over many hours. All of that stored energy is discharged in one enormous pulse that lasts for a fraction of a microsecond. The pulse creates a powerful electromagnetic field that slams a flyer plate into the deuterium



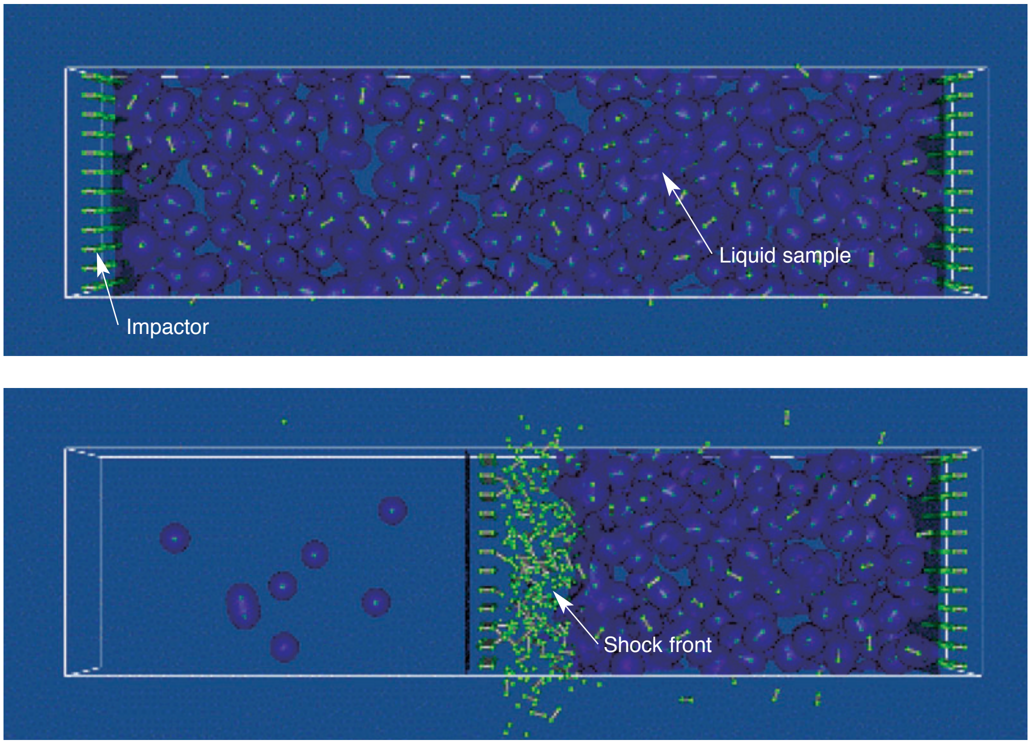
sample capsule. Sandia's magnetically driven plate is faster although smaller than the flyers used by Livermore's two-stage gas guns for shock experiments. It thus results in higher shock pressures. The *Z* accelerator also sustains a shock for a longer time than the Nova laser.

The two sets of experiments on the Nova laser showed that the deuterium samples were compressed to a density much higher than anyone had expected. These data differed from those used to predict the then-current model of the equation of state (EOS) for hydrogen and its isotopes. An EOS is a mathematical representation of a material's physical state as defined by its pressure, density, and either temperature or energy. It is a necessary constituent of all calculations involving material properties. Predictions concerning the formation and evolution of large planets, such as Jupiter, strongly depend on the EOS of hydrogen at pressures reached in the Nova experiments.

The *Z* flyer data reached pressures up to 70 gigapascals, which overlapped part of the pressure regime of the Nova laser experiments. The Nova experiments determined the EOS by using an x-ray probe and x-ray microscope to look into the deuterium as it was being shocked. The Sandia experiments simultaneously shocked a deuterium sample and a foil of aluminum. Researchers then found the EOS by comparing deuterium's behavior with that of aluminum. Although the Sandia EOS data required the comparison with aluminum, the *Z* flyer produced a shock in the deuterium that held a constant pressure for much longer than did the experiments with the Nova laser.

At a pressure of 40 gigapascals, the Nova and *Z* data agree, showing that the hydrogen EOS is about 20 percent more compressible than it was earlier thought to be. In other words, at this pressure, hydrogen will squeeze into a smaller volume with a higher density than previous models had predicted. At a pressure of 70 gigapascals, the Nova data show an even larger compressibility compared with equilibrium theory—almost 50 percent higher—while the *Z* flyer data are about 7 percent higher than theory predicted. "This is a considerable and important discrepancy," says Livermore physicist Robert Cauble, who oversaw the experiments on both the Nova laser and the *Z* accelerator.

Galli and Gygi performed two sets of simulations as they sought an explanation for the experimental results. The first simulations were of hydrogen under fixed pressure and temperature. The pressure values ranged from 20 to 120 gigapascals while temperatures ranged from 5,000 to 12,000 kelvins. Galli and Gygi then simulated the behavior of liquid deuterium during a shock experiment. Although the simulations of static conditions gave



Quantum simulations of shocked hydrogen reveal the atomic-scale structure of the shock front. (top) Thirteen hundred and twenty deuterium atoms are arranged in a periodically repeating molecular dynamic cell that contains an impactor, a wall, and a liquid sample. Four computer experiments used different impactor velocities in an effort to mimic experimental results. (bottom) The shock front and the compression of the deuterium atoms are shown from one computer experiment.

results that agreed with Sandia's data, the simulation of a shock in deuterium gave results that agreed with the Livermore Nova shocks.

Gygi notes that the conditions of the Nova and *Z* accelerator experiments differed. For one thing, the time scales of the pulse were different: 2 to 4 nanoseconds in Nova and about 30 nanoseconds in the *Z* machine. "Another variable may be that a laser beam is very different from a magnetic pulse," says Gygi.

Although the simulations did not supply a full explanation for the difference between the two sets of experimental results, Galli and Gygi's calculations did help to point out possible important differences. "In the past," says Gygi, "experimentalists with different results just pointed fingers at each other. Now, we hope that simulations will help to explain the physical reasons causing disagreement between different experiments. Also, big experiments are often expensive to repeat. The Nova laser is gone completely, so reproducing part of the Nova results with simulations can be very useful."

Water, Water Everywhere

Recent experiments also explored one of the most common liquids—water. "You would think that everybody knows everything about water," says Galli, "but that is far from the truth. And water is in practically everything in our world." Water is in many materials studied at Livermore: Biological systems are largely water, high explosives contain water, and water vapor may accumulate inside an aging nuclear weapon.

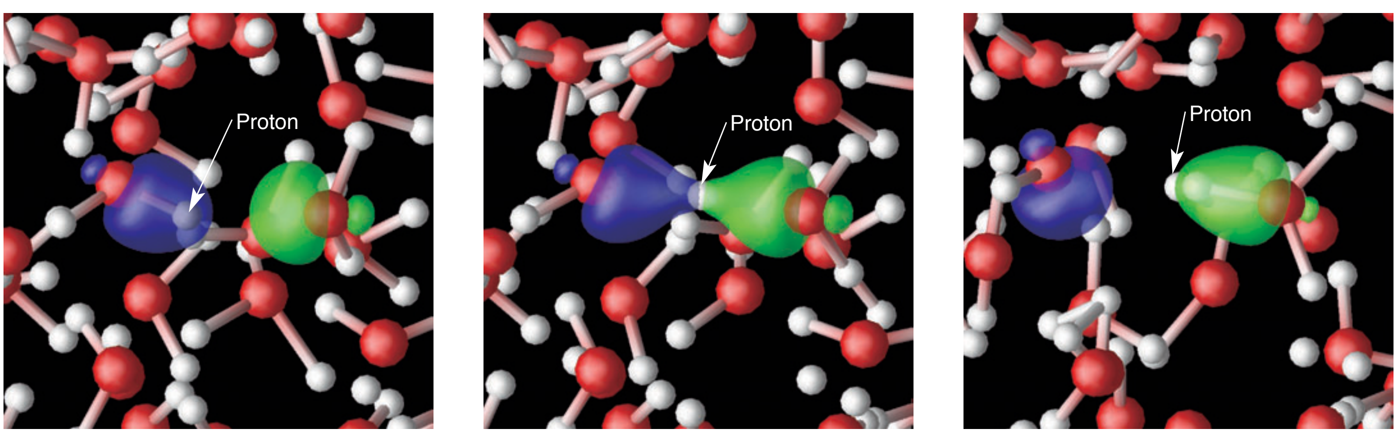
Physicist Eric Schwegler, Galli, and Gygi were interested in what happens to water under pressure, information important to Livermore's U.S. nuclear weapons stockpile stewardship mission. In particular, they were interested in learning how the water molecule comes apart under high-pressure conditions.

First, they developed a model of liquid water at ambient conditions, which compared favorably with recent x-ray data gathered at the University of California at Berkeley and with neutron diffraction data gathered in England. Then they modeled water at moderate pressure and found structural data that agreed with recent diamond anvil cell experiments performed at Commissariat à l'Énergie Atomique (CEA) in France.

Scientists already knew that under ambient conditions, water molecules rarely dissociate (come apart)—just once every 11 hours. When dissociation does occur, two water (H_2O) molecules become hydroxide (OH^-) and hydronium (H_3O^+), with one proton hopping to the other H_2O molecule. How increased pressure affects dissociation has long been debated.

Experiments on water at extreme temperatures and pressures have been few. One pioneering 1985 experiment at Livermore used a two-stage gas gun to shock water with pressures up to 26 gigapascals and temperatures to 1,700 kelvins. This experiment did not find any evidence of H_3O^+ under pressure. These data led to the suggestion that the dissociation mechanism at high pressures might be different from the one at ambient conditions, that perhaps a single H_2O molecule dissociates to H^+ and OH^-.

In quantum simulations of static pressure conditions ranging up to 30 gigapascals, Schwegler's team found that the dissociation process begins in earnest at 14 gigapascals. By 30 gigapascals, dissociation is occurring once every billionth of a second. The team was surprised to discover the same dissociation process that occurs at ambient conditions in which a proton jumps across to another water molecule. The simulations also indicated why the 1985 experiment did not reveal this process. At very high



Snapshots of the dissociation of a water molecule at high pressure. (left) As the water molecules dissociate, (middle) a proton is transferred to a neighboring water molecule so that (right) a hydroxide (OH^-) and a hydronium ion (H_3O^+) are formed.

pressures, the lifetime of a H_3O^+ molecule is on average only 9.8 trillionths of a second, too short to be observed in the 1985 experiment with detection technologies available then.

For Better Health

Schwegler, Galli, and Gygi are also working with researchers in Livermore's Biology and Biotechnology Research Program (BBRP) Directorate to simulate the dynamic behavior of DNA and other biomolecules. The goal is to combine Livermore's expertise in biology, simulation methods, and high-performance computing to nurture a new Laboratory core competency in computational biology. (See *S&TR*, April 2001, pp. 4–11.)

The simulations of water at ambient conditions were a necessary jumping-off point since all biomolecules contain a high percentage of water. Such liquid-phase simulations are far more complicated than those of isolated molecules in the gas phase because of the increased number of atoms that must be modeled.

"Getting water right made our future work much easier," says Schwegler. "And there are lots of experimental data to compare."

Subsequently, the team developed first-principles simulations of the dissolution of sodium and magnesium ions in water. In each case, their simulations agreed with numerous experimental investigations by others, but they also found several interesting features that had not been seen before.

That work was preparation for quantum simulations of the DNA sugar–phosphate backbone connecting the millions of base pairs that make up our genetic code. The flexibility of DNA in solution is central to the formation of DNA–protein complexes, which in turn mediate the replication, transcription, and packaging of DNA. Part of this flexibility comes from rotations around the bonds found in the

Simulating Quantum Molecular Dynamics

In the classical molecular dynamics approach, a model of interactions between atoms is supplied as input before a simulation can be carried out. Such models are based on a priori knowledge of the physical system being studied. "Those models work if you know the chemical bonds already," says physicist Francois Gygi.

In contrast, first-principles, or ab initio, molecular dynamics does not require any a priori knowledge of interatomic interactions. These simulations use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. The existence of chemical bonds is the result of electron interactions and the laws of quantum mechanics. Quantum simulations can describe the forming and breaking of chemical bonds, which cannot be done using classical molecular dynamics. Thus, classical molecular dynamics cannot explain complex states of matter such as hot, compressed fluids in which molecules come apart and regroup. Quantum molecular dynamics, however, is an ideal method for showing what happens to fluids under pressure.

The fundamental physics equations that must be solved in quantum simulations are extraordinarily complex. Until powerful computers such as Livermore's ASCI White came along, ab initio quantum molecular dynamics simulations could handle only a few atoms. Even now, a model of a few hundred atoms over less than a millionth of a second takes days of computing time to complete on Livermore's huge computers.

Modeling the behavior of molecules at the quantum level requires not only unprecedented computational power and speed but also specially designed simulation codes. One such code is JEEP, which Gygi began developing when he was at the Swiss Federal Institute of Technology.

JEEP is based on density functional theory, which describes the electronic density of a molecular or condensed system. Walter Kohn of the University of California at Santa Barbara won the Nobel Prize for Chemistry in 1998 for his development of density functional theory. In its original form, this theory was confined to ground-state properties of molecules. Since then, it has been expanded and made applicable to the study of atomic motion and complex dynamic effects of matter. Kohn's work on density functional theory has revolutionized the way scientists approach the electronic structure of atoms, molecules, and solid materials in physics, chemistry, and materials science.

Since coming to Livermore, Gygi has adapted and optimized JEEP for use on the massively parallel computers of ASCI. Now, with ASCI computers, he can examine materials systems with hundreds of atoms and thousands of electrons extremely accurately.

Monte Carlo codes are more accurate but have been extremely demanding of computing time. Every increase in the number of particles (N) being modeled requires N^3 more computing time. Twice as many electrons requires 8 times more computing time, 3 times as many electrons requires 27 times more computing time, 4 times as many electrons requires 128 times more computing time, and so on. Modeling more than a few atoms requires prohibitively long periods of computing time. Recently, however, physicists Andrew Williamson, Jeff Grossman, and Randy Hood developed a technique that allows for linear scaling of computing time for quantum Monte Carlo calculations. In other words, doubling the number of electrons only increases computing time by a factor of two instead of a factor of eight. This important breakthrough is based on techniques also used in some quantum molecular dynamics codes.

backbone.

To learn more about how these rotations work, the team modeled the smallest part of the DNA backbone, the dimethyl phosphate anion (DMP^-). They observed changes in the shape of DMP^- when it was exposed to a sodium cation, changes that had not been seen in any previous classical molecular dynamics simulation of DMP^- in water. In future simulations, they plan to examine the influence of magnesium and other cations on the shape and flexibility of DNA.

Schwegler's team has also been collaborating on studies of cancer-fighting drugs known as phosphoramides being done by Mike Colvin and his associates in BBRP. These nitrogen-mustard-based drugs have been used to treat cancer for 50 years, so there is plenty of experimental data to compare with simulations. By examining how the phosphoramide molecules are activated, this team hopes to find ways to improve the drug and to make it more effective. (See *S&TR*, April 2001, pp. 9–10.)

Mustard drugs are believed to work by forming cross-links between the two strands of a cancer cell's DNA. Because the cell cannot easily eliminate the cross-links, the cell cannot replicate itself and dies. Before the drug can attach itself to the cancer cell's DNA, it has to lose chlorine ions. With his quantum simulations, Schwegler is learning more about the activation process, examining how the drug loses the chlorine ions and how much energy is required.

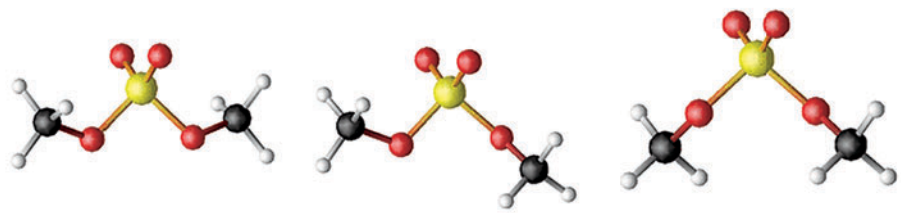
Surface Chemistry Is Key

Livermore researchers used both density functional theory (on which the JEEP code is based) and quantum Monte Carlo codes to perform first-principles calculations of silicon nanoclusters, or quantum dots, which are tiny silicon molecules just a few nanometers in size, about 100,000 times smaller than the width of a human hair. These nanoclusters produce different colors of light depending on their diameter and are being considered as replacements for the fluorescent markers that researchers now use to tag proteins during experiments. With the markers, scientists can locate specific proteins and watch them as they go about their business.

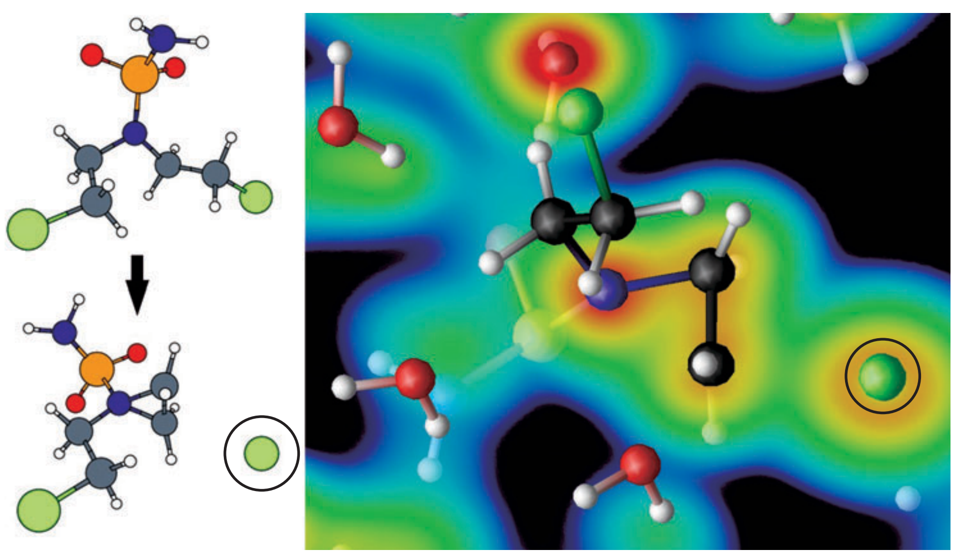
Existing fluorescent dyes work well as markers. But they are short-lived. Their fluorescence rapidly fades until they are no longer detectable. They also have to be excited by a specific wavelength of laser light that matches their absorption. If researchers are studying more than one protein at a time and use multiple fluorescent markers, they must also use as many lasers as there are different markers.

Silicon quantum dots have several advantages as biomarkers. They do not bleach out, and multiple markers can be excited by a single laser. "Given their small size, they would be a gnat on the side of a protein," says Williamson, "and the protein should continue to act and react normally."

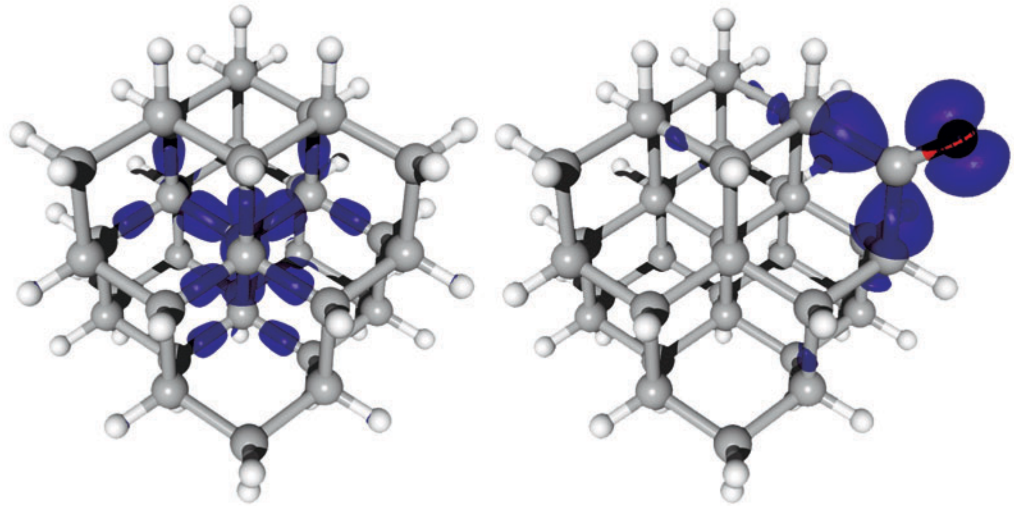
The synthesis of silicon dots is still in its infancy. Livermore has several experimental efforts under way to synthesize them. A long-term goal is



Part of the flexibility in DNA comes from rotations around the bonds found in the backbone, which consists of deoxyriboses linked together by phosphodiester bridges. Shown here is a simple model of the phosphodiester linkage found in the backbone of DNA. The molecule can adopt a variety of conformations by rotations around the phosphorus–oxygen bonds.



The cyclization of phosphoramide mustard in solution. (left) As the new carbon–nitrogen bond is formed, a chloride ion (circled) leaves the mustard and (right) is solvated by the surrounding water molecules.



(left) In a 71-atom silicon quantum dot, the white atoms are hydrogen atoms bonded to the surface that are "passivating" the dot and making it less reactive. A silicon dot that is completely passivated by hydrogen will have all its electrons in the center. (right) When two of the hydrogen atoms are replaced by a more reactive oxygen atom, the electron charge cloud is drawn toward the oxygen atom. This dramatically changes the optical properties (wavelength) of the silicon quantum dot.

to use silicon nanoparticles in biosensors to detect biological and chemical warfare agents.

During the manufacture of the quantum dots, contamination is a concern. Oxygen, especially, can be a killer for silicon, notes Williamson. Recent Livermore simulations examined the effect of oxygen on silicon particles. A single oxygen atom, as well as many other contaminants, can make a big difference on a quantum dot because of the dot's large ratio of surface area to volume. Surface chemistry plays a big role in the study of these tiny particles.

The effects of surface chemistry are illustrated in the figure above. The left portion of the figure shows a nanometer-size silicon quantum dot made up of 71 atoms. The white atoms on the surface are hydrogen atoms bonded to the dot in such a way as to "passivate" the surface. This means they attach themselves to the highly reactive surface silicon atoms (gray). The purple cloud shows the region where the electrons that will absorb light are most likely to be located in this silicon quantum dot. For a silicon dot completely passivated by hydrogen, the electrons are located in the center of the dot. The right portion of the figure above shows how the situation changes when two of the hydrogen atoms are replaced by a more reactive oxygen atom. The electron charge cloud is drawn toward the oxygen atom, and this change in the electron density dramatically changes the optical properties of the silicon dot.

The team is currently broadening the scope of its nanostructure investigations to include other semiconductor materials such as germanium and cadmium–selenide.

Bigger and Better

One goal of Galli's group for the next few years is to apply quantum simulations to a wider and broader set of problems and to use quantum simulations on a par with laboratory experiments as a tool for research in science and engineering. Quantum simulations are a fully predictive approach that will provide a new window through which scientists can observe the world at the atomistic level in exquisite detail, avoiding uncontrolled approximations. Galli's group will focus on fluids under extreme conditions—for example, water under shocked conditions—and on building knowledge and expertise in the field of nanoscience, in particular, modeling artificial and biological nanostructures for labeling and sensing applications.

Because of the success of their quantum simulations, Galli and Gygi are working with IBM on the design of the next-generation ASCI computers. When these monster computers arrive, extremely complex simulations may be able to answer questions that cannot now be answered.

—*Katie Walter*

Key Words: hydrogen, JEEP, nanostructures, quantum dots, quantum molecular dynamics, quantum Monte Carlo calculations, quantum simulations, water.

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Building a Virtual Telescope

A new three-dimensional code simulates for the first time the structure and evolution of stars.

In the Egyptian pantheon, Djehuty was the guide to heaven, earth, and the netherworld; lord of calculation, wisdom, and judgment; and protector of knowledge, mathematics, and science. It seemed appropriate, then, for Lawrence Livermore astrophysicists David Dearborn and Peter Eggleton to take his name for their breakthrough three-dimensional code that simulates the evolution and structure of stars.

The physical processes of stars have long been of interest to Livermore researchers because understanding the prime mechanism of stellar energy—thermonuclear fusion—is part of the Laboratory's national security mission. "Stars are high-energy-density ovens," says Dearborn. "Several Laboratory programs are interested in the properties of stars, and many Livermore physicists have backgrounds in astrophysics."

Dearborn points out that stars provide the standards of reference for measuring the size, age, chemical composition, and evolution of the universe. Stars have also been used as physics laboratories

The Egyptian god Djehuty was the guide to heaven, earth, and the netherworld; lord of calculation, wisdom, and judgment; and protector of knowledge, mathematics, and science. His image is seen in many hieroglyphic tablets.

that strengthen our understanding of complex physical processes. For example, they have been used to better understand the properties of hot plasmas as well as fundamental particles such as neutrinos. Stars have also been used to suggest the properties of exotic particles such as axions, which have been proposed to explain why the universe contains more matter than antimatter.

Eggleton notes that scientific knowledge of stars may appear to be mature, but in fact, much of what we know about stars—especially the way they generate energy and how they evolve from a dust cloud to a supernova or red giant—may well be significantly incomplete. "We need to improve our knowledge about stars," he says.

The reason for the imperfect understanding is that many stellar processes are complex, three-dimensional phenomena that have been modeled only in coarse approximation using one-dimensional computer codes. For example, the transport of energy through a star by convection from its superhot core is a three-dimensional process, which limits the value of one-dimensional calculations, even for perfectly spherical stars. (See the box on pp. 6–7.) Although a one-dimensional convection simulation could be inaccurate by only 10 percent at any moment in time, such "small" errors can easily accumulate over time. The result might be a final discrepancy of 100 to 200 percent in some properties calculated for such stellar objects as Cepheids, which are large, pulsating stars often used to calculate the distance scale of the local universe.

Need for 3D Codes

Convection is only one of many stellar phenomena that require a three-dimensional simulation code for accurate modeling. Other complex phenomena that astrophysicists have long desired to simulate include the evolution of elements created in a star, the preexplosion structure of supernovas, and the physics of binary stars, which comprise nearly half of the visible mass of the universe.

Dearborn says that developing a three-dimensional code to realistically model stars is challenging for even the most accomplished teams of computer scientists and astrophysicists. Before Djehuty, three-dimensional stellar models were limited to about 1 million zones. (Computer simulations divide an object into numerous small cells, or zones, whose behavior is governed by sets of physics equations. The totality of the zones, or cells, is called a mesh.) The million zones represent only modest segments of a star. Moreover, the simplified models did not incorporate all the physics pertinent to a star's core where nuclear energy is produced, and they did not simulate gravity in a realistic manner. "While the earlier codes are important starts toward improving our understanding, it is clear that the solutions to some problems necessitate whole-star modeling," Eggleton says.

The advent of massively parallel computing, wherein computers have hundreds and even thousands of processors, and Livermore's participation in the National Nuclear Security Administration's Stockpile Stewardship Program—to assure the safety and reliability of the nation's nuclear stockpile—led Livermore scientists to gain expertise in supercomputers and parallel codes. Along with astrophysicist Kem Cook, Dearborn and Eggleton saw that Livermore was becoming a uniquely qualified institution to move the calculation of stellar properties to a higher level of understanding. In particular, they saw that one element of stockpile stewardship, which uses massively parallel computing techniques to simulate the performance of nuclear warheads and bombs in a program called Advanced Simulation and Computing (ASCI), would be pertinent to their quest for a whole-star, three-dimensional model.

Dearborn and Eggleton's vision was to take advantage of Livermore's expertise in ASCI computations, code and algorithm development for massively parallel computers, astrophysics, high-energy-density physical data and processes, and experience in interdisciplinary coordination to attack the fundamental questions of stellar structure and evolution.

A Laboratory-Wide Team

In 1999, Dearborn and Eggleton assembled a team to develop Djehuty as a three-year Strategic Initiative under Laboratory Directed Research and Development funding. The collaboration has included John Castor, Steven Murray, and Grant Bazan from the Defense and Nuclear Technologies Directorate; Kem Cook from the Physics and Advanced Technologies Directorate; Don Dossa and Peter Eltgroth from the Computation Directorate's Center for Applied Scientific Computing; and several other contributors. "Collaboration from throughout the Laboratory has been essential in this project," says Dearborn.

The team designed Djehuty to operate on massively parallel machines with the best available physical data about stars and with algorithms tailored specifically for the massively parallel environment. Notes Dearborn, "There's been tremendous work at the Laboratory in developing parallel codes and learning how to do calculations in a manner that won't bog down the machines." The code development process involved assembling and reconfiguring a number of Livermore codes that already existed, many of them parts of unclassified software belonging to the ASCI program, and optimizing them for astrophysical simulations.

Djehuty also takes advantage of the Laboratory's significant knowledge about opacity (a measure of the distance photons at a particular frequency travel through a particular material) and equations of state (the relationship between a material's pressure, temperature, and volume). Opacity and equation of state are two key pieces of data that are used in stockpile stewardship work for studying matter under extreme conditions. In that respect, says Dearborn, developing Djehuty is well aligned with Livermore's programmatic interests that focus on understanding high-temperature physics and performing numerical simulations of complex physical reactions.

The code currently features accurate representations of different elements' equations of state, opacities, radiative diffusion transport (how photons are absorbed and reemitted when they interact with atoms and electrons in a star's interior), and nuclear reaction network (fusion reaction rates and abundance of species formed). Finally, Djehuty features a gravity package for spherical stars, a provision that is being improved significantly so it will be

Probing the Interiors of Stars

Stars, unlike planets, produce their own energy and do so by thermonuclear fusion. Much of the complexity underlying the computer code Djehuty, Livermore's three-dimensional code for star structure and evolution, is its realistic simulation of fusion, which converts hydrogen nuclei into helium ions. The process is often called hydrogen burning and is responsible for a star's luminosity.

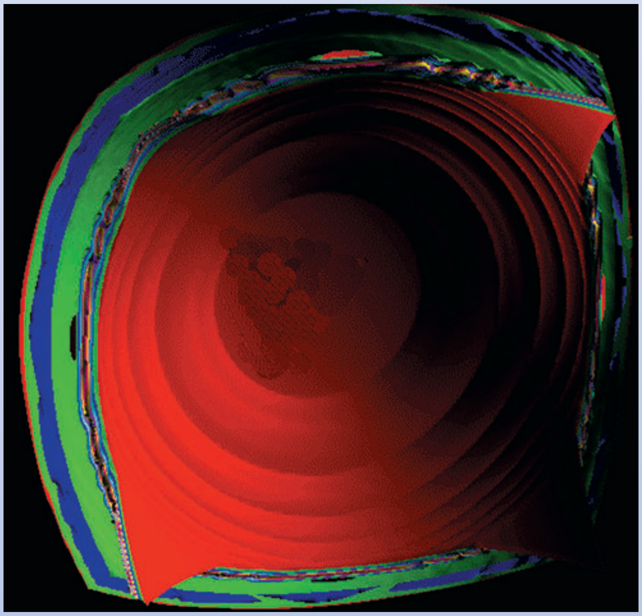
Fusion reactions occur in the core, the innermost part of the star. In a star about the size of our Sun, the hydrogen fuel is eventually consumed after billions of years. The core slowly starts to collapse to become a white dwarf while the envelope expands to become a red giant. Our Sun will reach this stage in about 5 billion years.

In contrast, the core of a star larger than the Sun is driven by a complex carbon–nitrogen–oxygen cycle that converts hydrogen to helium. In these massive stars' cores, hot gases rise toward the surface, and cool gases fall back in a circulatory pattern known as convection. After depleting its hydrogen—and subsequently its helium, carbon, and oxygen—the contracting core of a massive star becomes unstable and implodes while the other layers explode as a supernova. The imploding core may first become a neutron star and, later, a pulsar or black hole.

The cores of stars are turbulent in a manner analogous to a boiling kettle, says Livermore astrophysicist Peter Eggleton. Driven by enormous heat, the material in a core takes about a month to completely circulate (our Sun accomplishes it in about two weeks). "One-dimensional simulations give you an average of what's going on in the kettle instead of telling you what's happening on a second-to-second basis, so we are forced to make some bold assumptions." Eggleton also says that one-dimensional codes cannot model time-dependent convection in such events as helium flashes, which occur in the late stages of a red giant star.

One of the long-standing issues of astrophysics has been determining the correct convective core size of stars. Astronomical observations have suggested that the convection region is larger than has been assumed since the 19th century. Astronomers call the situation convective-core overshoot, meaning that the core probably extends beyond the long-accepted boundary.

Determining the exact size of the convective core is of more than passing interest. If the core is indeed larger than has been assumed, then stars could be much older than has been believed, which has profound implications for how the universe evolved and its real age. "The modeling of convection is one of the weakest points in our

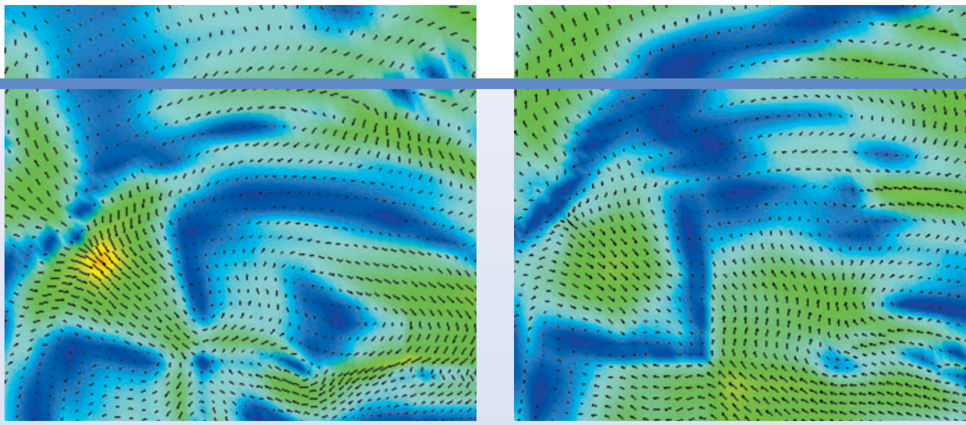


When low-mass stars such as our Sun become red giants, they grow a helium core. Eventually the helium core ignites and begins burning to carbon and oxygen. The ignition begins in a shell that initially expands and drives a weak shock into and out of the star. The image shows the velocity contours of the expanding shell in a cutaway segment of a star in which ignition is beginning. The red areas represent the highest velocity, corresponding to the rapidly expanding shell both in front and in back (barely visible).

possible to simulate a host of aspherical stellar objects.

The First Simulation

The team's early strategy was to test the code's accuracy and achieve some optimization of it. In September 2000, using the 680-gigaops (billion calculations per second) TeraCluster 2000 (TC2K) parallel supercomputer at Livermore, the team successfully executed a three-dimensional simulation of a star. This was the first three-dimensional simulation of an entire star, but it ran on just one of TC2K's 512 processors, using only some of the code's physics on a modest mesh containing approximately 400,000 cubic zones. "Our first models were too small to accurately represent a star's structure, but they were sufficient to study different zone mesh structures and to optimize the physics equations we were using," says Dearborn.



Two simulations taken about 8 minutes apart show the changes inside the core of a star four times the mass of our Sun. Colors represent relative velocity (increasing from blue to yellow), and the arrows show the direction of convective currents.

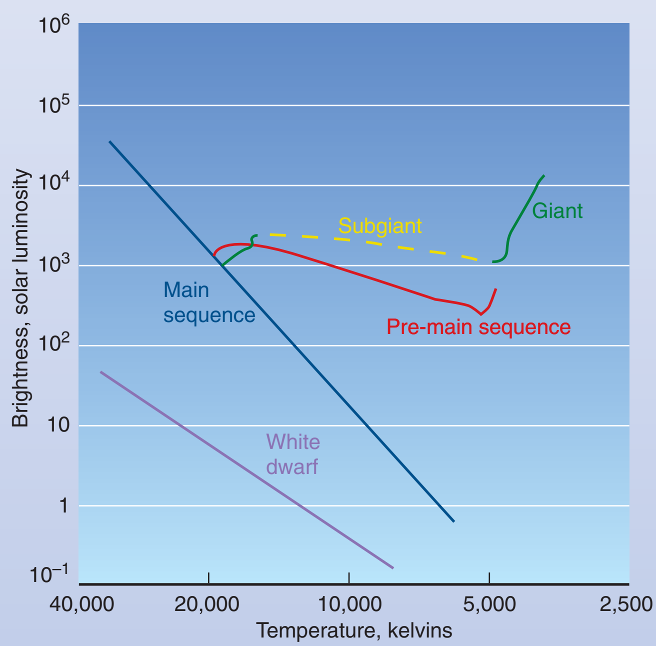
understanding of stellar structure and evolution," says Livermore astrophysicist David Dearborn.

The issue over the size of the convection region is serving as a way to verify and validate the accuracy of Djehuty. The code development team made convective core overshoot a priority in part because the fusion process occurs during the earliest and simplest phase of stellar evolution—during what is called the main sequence. The main sequence is shown on a Hertzsprung–Russell diagram, which plots stars' temperatures versus their brightness, thereby showing their evolution.

"Observations assure us that our best one-dimensional approximations of convection are flawed," says Eggleton. "With Djehuty, we have a three-dimensional code with accurate physics to determine what exactly happens in the core. There are big rivers flowing in stars' cores, and we want to follow them."

One simulation modeled a star early in its evolution, prior to its joining the main sequence. As expected, it did not show any convection motions from thermonuclear fusion. Another simulation studied a massive star that had just reached the main sequence and so witnessed the onset of convective motion from fusion. A third simulation looked at a red giant, a very old star that possesses a large core of helium. The helium eventually ignites in what is called a helium flash.

The simulations suggested that a star's convective core indeed exceeds its classical boundary. Additional computationally intense simulations, each requiring a month of supercomputer time, will be done this year to model a star's convective core at key stages in its lifetime.



The Hertzsprung–Russell diagram plots the temperatures of stars versus their brightness and is useful for plotting their evolution. This diagram follows a star with six times the mass of our Sun. The star spends most of its lifetime in the main sequence, characterized by producing fusion in its inner core. Djehuty simulations are modeling stars in every phase of their evolution.

Satisfied with the early simulations on one processor, the team then modified the code to run in a massively parallel computing environment. "It's a big transition going from one to many processors because we need at least 10 million zones to model an entire star," says Dearborn. Fortunately, he says, Livermore has invested significant resources to figure out how to break up a complex physics problem, such as following fusion reactions in time, for efficient processing by hundreds and even thousands of processors.

Generating and monitoring large three-dimensional meshes containing millions of zones is a huge task. To aid computing, the Djehuty team constructs a mesh sphere of seven blocks: one in the center and six surrounding it. The outlying six are distorted at their outer edges to make them spherical. Each block contains at least 1 million zones. Each zone represents thousands of kilometers on a side, and several thousand zones are assigned to a processor. All the processors must communicate efficiently with each other simultaneously. The key to Djehuty's simulation power is its ability to access many processors to efficiently compute the physics in each of the millions of zones. "We're fortunate to have so many people who can develop a code like this," says Dearborn.

The team has run simulations on increasing numbers of processors on the TC2K. Several simulations, using 128 processors and 56-million-zone meshes, were some of the largest astrophysics calculations ever performed; they generated close to a terabyte (trillion bytes) of data. The team has also begun to perform simulations on Livermore's ASCI Frost, the unclassified portion of ASCI White, currently the world's most powerful supercomputer. Simulations on ASCI Frost have used 128 of that machine's processors to evolve stars with 60-million-zone meshes.

With the code running satisfactorily in a massively parallel environment, Dearborn and Eggleton focused on resolving a long-standing controversy in astrophysics. That controversy surrounds the discrepancy between the results from one-dimensional stellar models and data gained from astronomical observations concerning the size of the convection region inside a star. (See the box on pp. 6–7.) This region is where hot plumes of gas rise and fall. The team has simulated the cores of several stars, ranging from young stars before the onset of fusion reactions to old stars about half the age of the universe. Eggleton says that one-dimensional computer models are especially incomplete in simulating late stellar evolution, which is often characterized by deep mixing of gases and sudden pulses of energy.

Virtual Telescope at Work

Eggleton compares Djehuty to a kind of virtual telescope that can take snapshots during a star's lifetime of several billion years and examine in detail the star's structure and the various physical processes at play. "There is no comparable three-dimensional code, although there have been heroic efforts to develop one," he says. As a result of the early simulations, the Livermore team anticipates being able to accurately model in three dimensions, for the first time, a host of important stellar objects. For example, Djehuty will be vital to understanding supernovas, the brightest objects in the universe, and about which much is unknown, as well as Cepheids.

Dearborn predicts that Djehuty will provide an important link between theory and observation that will further our knowledge of stellar structure and evolution. Livermore's Stefan Keller is conducting a number of observational studies to verify the Dhejuty simulations. One study uses a certain population of Cepheids to observationally determine the relationship between mass and luminosity that is dependent on the original amount of mixing in the star's convective core. Preliminary results indicate that these Cepheids are considerably more luminous than predicted by standard one-dimensional models, a result suggesting a larger

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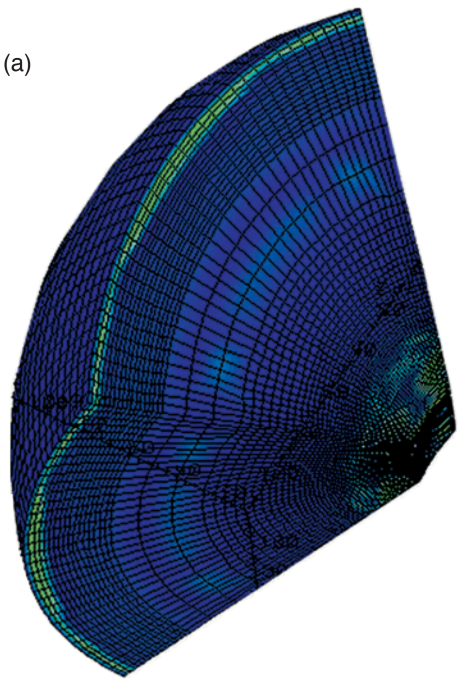

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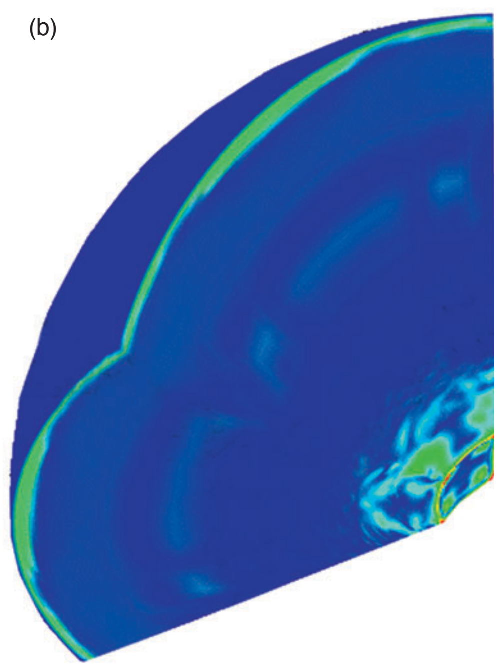
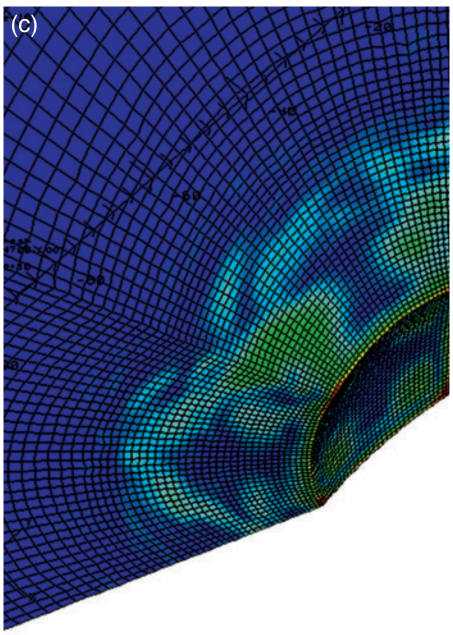


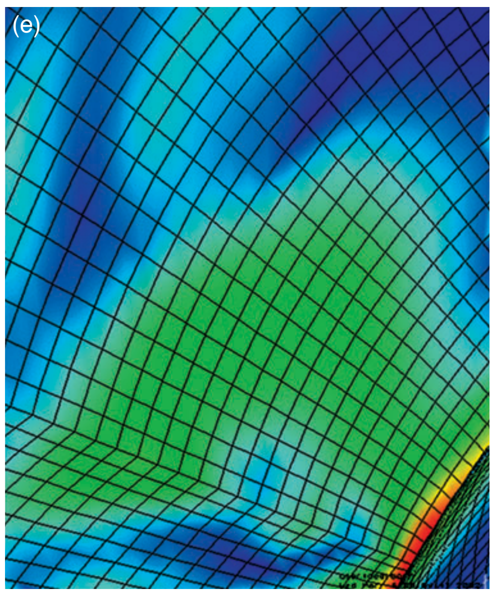
degree of mixing than was previously thought. Djehuty simulations appear to confirm the observations.

In another study, astrophysicist Rob Cavallo is observing variations in the surface abundances of some elements in evolved red giant stars. The variations are caused by some form of nonconvective mixing process, which can only be determined with the use of a fully three-dimentional code such as Djehuty.

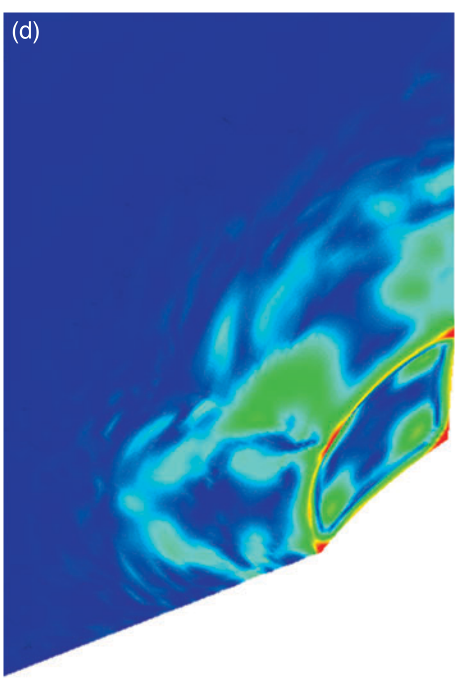
The team is also working to improve the code and better interpret its output. One goal is improving the accuracy of opacities. "There are a range of problems where a star's behavior depends on the opacity of material whose composition is rapidly changing," says Dearborn. The team plans to attack those problems by permitting the code to generate opacity levels using OPAL, a database of stellar opacity that was developed at Livermore several years ago. (See *S&TR*, April 1999, pp. 10–17.)

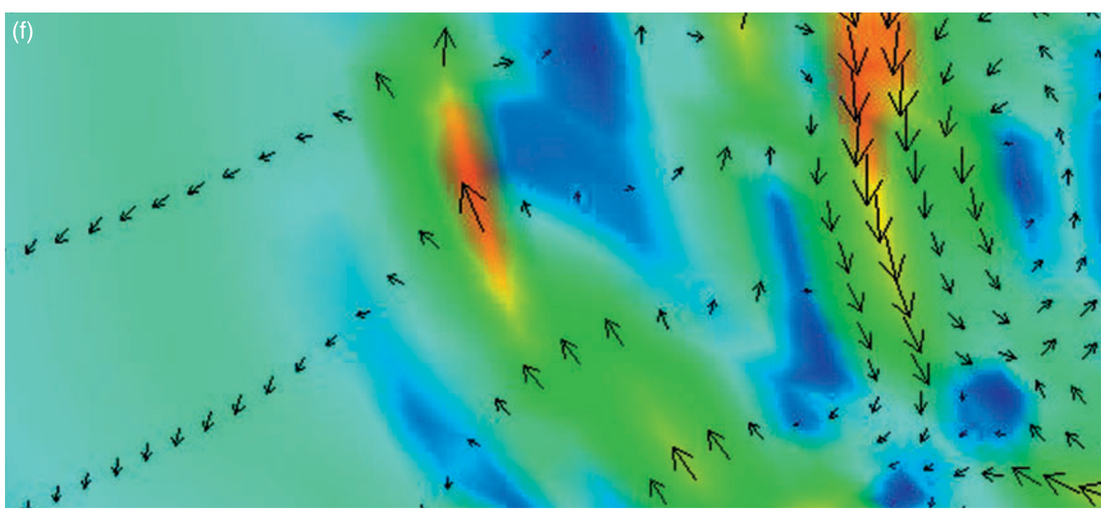
Another task is improving the techniques to better visualize and thereby understand the vast amounts of data generated by Djehuty. Analysis and visualization are the key for turning huge numerical simulations into scientific understanding, says Dearborn, and at present, "We must improve our ability to analyze three-dimensional structures. With longer, larger, and





Increasingly magnified sections of a star with four times the mass of the Sun can be seen in these Djehuty simulations. Here, (a) and (c) are the same as (b) and (d), respectively, but show the location of mesh zones. A closeup of the star's convective core is shown in (e). Colors represent relative velocity (increasing from blue to yellow). The bulk of motion lies in the core, where convection currents driven by carbon–nitrogen–oxygen burning occur. The areas of convection appear to extend beyond what one-dimensional models depict, but Djehuty's models are consistent with recent astronomical observations. (f) A two-dimensional slice of a Djehuty three-dimensional simulation depicting convection currents deep inside the core. The arrows signify the directions of the currents.





more realistic simulations, we must develop better tools to analyze our simulations to extract the greatest amount of information. We can't eyeball 10 million zones in three dimensions. We must have ways for a computer to look for irregularities and flag them."

Recently, the team began using MeshTV, a program that was designed at Livermore to visualize data for three-dimensional meshes. MeshTV can display an animation of data changing over time and permit a user to rotate, zoom, or pan an object while a movie assembled from the data is playing. (See *S&TR*, October 2000, pp. 4–12.)

A Continual Code Development

Djehuty development will never be finished, although it will eventually become much less a development code and more a production code ready for use. The team continues to enhance Djehuty's physics and refine its algorithms. Development is also under way to permit simulation of rapidly rotating stars and, in particular, binaries. Binary stars revolve around a common center of gravity and sometimes exchange some of their mass or even merge into one star. Often, one binary is distorted by the gravitational pull of the other, and the result is seen in varying brightness.

"Simulating binaries has become our main physics priority," says Dearborn. "We want to see how mass comes off one star and is absorbed by the other." One-dimensional codes don't work for binaries because when two stars interact, the problem is three-dimensional.

Binary simulations require a more accurate means to simulate gravity, one that automatically changes to reflect a star's size, shape, and internal physics. Once this enhanced gravity treatment is incorporated into Djehuty, the code will be able to represent binaries as well as stellar objects that are not perfectly spherical. "Once work on binaries begins," says Dearborn, "we will enter completely new territory because calculations so far have been very crude."

The Livermore effort to revolutionize stellar evolution and modeling calculations has been well received at two international conferences. The enthusiasm generated by this work has led to two proposals to the National Aeronautics and Space Administration from U.S. academic researchers interested in collaborating with the Djehuty team on binary star evolution. Other researchers have proposed using the code to study white dwarfs, the phase of stellar evolution that occurs late in stars' lifetimes, depending upon their starting masses. Dearborn and Eggleton have also received inquiries about the possibility of modifying the code to run simulations of large planets and brown dwarfs.

Several postdoctoral scientists and university students have joined the Djehuty development team. With a user manual recently completed, the team is seeking university collaborators, both graduate students and visiting scientists, who would visit for several months at a time and join in astrophysical research that can be done nowhere else.

Dearborn and Eggleton hope to see a user facility established at the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (IGPP). The Livermore IGPP currently collaborates with all UC campuses, more than thirty U.S. universities, and more than twenty international universities. "Djehuty is a unique institutional asset for attracting astronomers and physicists interested in stars and what can be learned from them," says Eggleton.

—Arnie Heller

Key Words: Advanced Simulation and Computing (ASCI), ASCI Frost, ASCI White, binary stars, brown dwarfs, Cepheids, convective core, Djehuty, helium flash, Hertzsprung–Russell diagram, Institute of Geophysics and Planetary Physics (IGPP), Mesh TV, stellar evolution, supernovas, TeraCluster 2000 (TC2K), white dwarfs.

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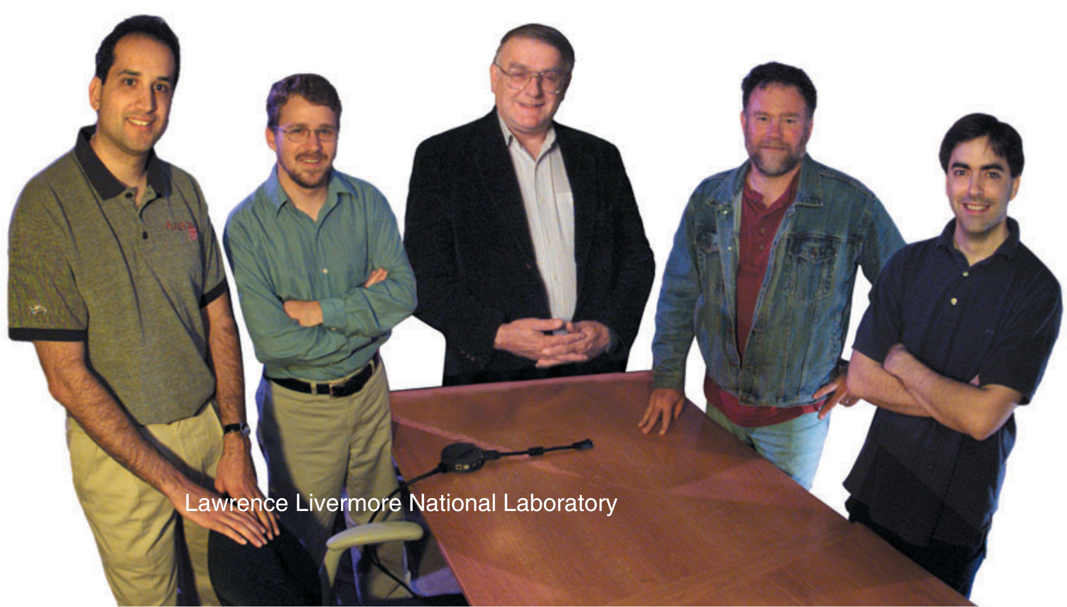
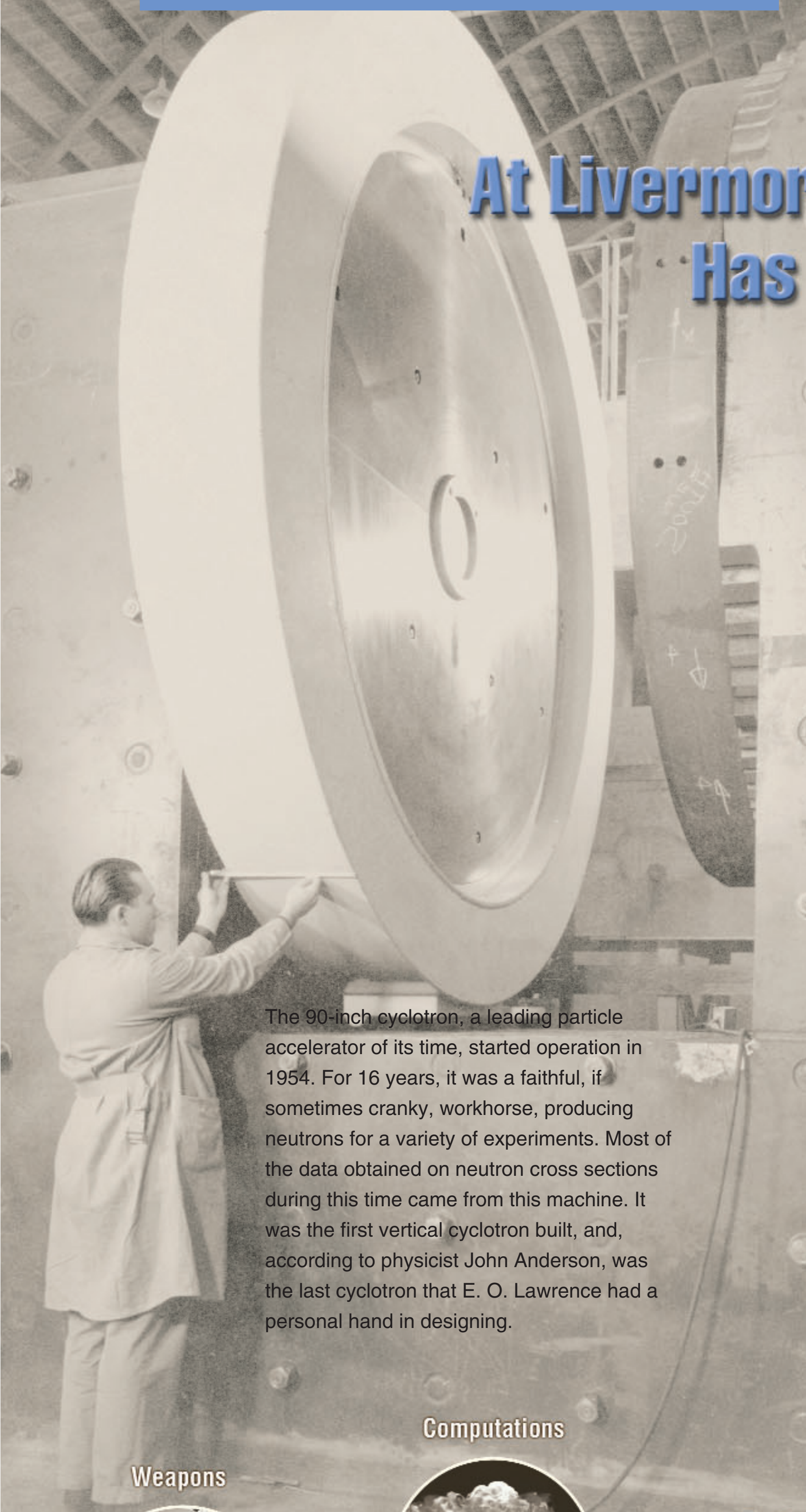


Some postdoctoral scientists and the project leaders on the Djehuty development team. From left, Rob Cavallo, Stefan Keller, team leaders Peter Eggleton and David Dearborn, and Sylvain Turcotte.



At Livermore, Audacious Physics Has Thrived for 50 Years

WHEN E. O. Lawrence selected Herbert York, a young physicist from Lawrence's Radiation Laboratory at Berkeley, to head the laboratory at Livermore, York had to come up with a starting point for possible programs, organization, and personnel at Livermore. The plan York developed called for four activities: thermonuclear weapons design, design and development of diagnostics for weapons experiments for both Los Alamos and Livermore, work on controlled thermonuclear reactions (in other words, fusion) for potential power sources, and basic physics research. All of these activities are, at heart, issues of physics. To understand the inner forces that govern a nuclear weapon, a fusion power source, or, indeed, the interior of a star requires knowing how the thermonuclear process works.

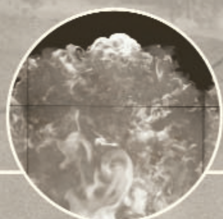
From the Laboratory's earliest days, physicists have explored some of the most difficult issues in the highly specialized fields of nuclear, condensed-matter, plasma, atomic, and molecular physics. As a result, the physics organization has always been a testing ground for new concepts and an integral contributor to major Laboratory programs, many of which it helped create.

> *"Every great advance in science has issued from a new audacity of imagination."*
>
> *John Dewey, philosopher*

The 90-inch cyclotron, a leading particle accelerator of its time, started operation in 1954. For 16 years, it was a faithful, if sometimes cranky, workhorse, producing neutrons for a variety of experiments. Most of the data obtained on neutron cross sections during this time came from this machine. It was the first vertical cyclotron built, and, according to physicist John Anderson, was the last cyclotron that E. O. Lawrence had a personal hand in designing.

Weapons

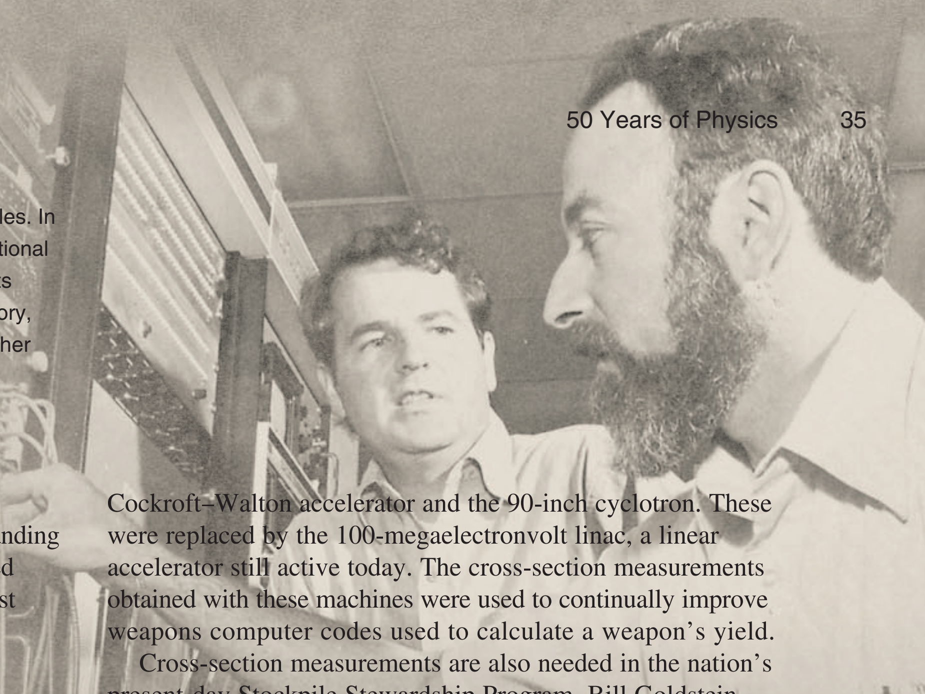
Computations



Engineering

Physics

Chemistry & Materials Science



The Laboratory has always been interested in astrophysics puzzles. In the 1960s, Laboratory physicists authored key papers on gravitational collapse and supernova explosions. In 1976, Livermore physicists John Browne (left), now director of Los Alamos National Laboratory, and Barry Berman used the Livermore's linear accelerator to gather key data to revise estimates of the age of the universe.

From their initial focus on the thermonuclear process, the Laboratory's physicists have advanced theoretical understanding and spearheaded breakthrough after breakthrough in applied physics—from the inner workings of the atom to the farthest reaches of the universe.

Exploring the Heart of a Weapon

Understanding a weapon's performance requires a thorough understanding of the properties of matter at extreme conditions—up to stellar temperatures and pressures—and of the interaction of matter with intense radiation. From the first days at Livermore, physicists made it their goal to better measure and validate material properties such as equations of state, opacities, and nuclear cross sections for these unique environments. Their tools included accelerators, gas guns, nuclear reactors, lasers, and nuclear tests on the one hand and advances in theory, powerful computers, and physics simulation codes on the other.

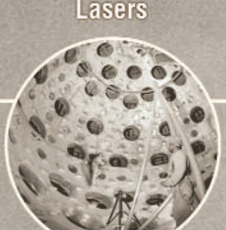
The nuclear cross section is particularly important for understanding how well a nuclear weapon performs; it has been of interest to the Laboratory from the start. The cross section is a measure of how likely it is that a particular reaction will occur between a nucleus of a particular material and an impinging particle. For nuclear weapons research, the particle of interest is usually a neutron, and the material is uranium, plutonium, steel—any of the materials that go into a nuclear device. Physicist John Anderson, who came to the Laboratory in 1956 and was associate director for Physics from 1978 to 1983, remembers, "In the 1950s, neutron physics was a hot topic. Many places were researching cross sections, but Los Alamos and Livermore were the only ones generating information applicable to weapons." Early Livermore physicists used two machines for gathering cross-section measurements: a Cockroft–Walton accelerator and the 90-inch cyclotron. These were replaced by the 100-megaelectronvolt linac, a linear accelerator still active today. The cross-section measurements obtained with these machines were used to continually improve weapons computer codes used to calculate a weapon's yield.

Cross-section measurements are also needed in the nation's present-day Stockpile Stewardship Program. Bill Goldstein, associate director for Physics and Advanced Technologies (PAT), explains, "One of the directorate's primary stockpile stewardship responsibilities is to support the Physical Data Research Program by providing validated data on material properties that are basic to weapons research." Just as in the past, physicists combine theory with computer simulations and laboratory measurements to provide the validated data needed for nuclear weapons simulations. With today's sophisticated tools, researchers can revisit some of the more difficult problems, reevaluating and refining measurements. One such example is a cross section in which a neutron smashes into a plutonium-239 atom, resulting in one plutonium-238 atom and two neutrons. Getting a good value for this cross section is particularly important because the production of plutonium-238 by neutrons is a major diagnostic for interpreting the results of past underground nuclear tests. For more than 40 years, large uncertainties in this cross section's value have limited the usefulness of plutonium-238 production as a nuclear test diagnostic.

In 2001, a five-year collaboration between Livermore and Los Alamos produced new measurements of this crucial reaction. The Livermore team, led by physicist John Becker, developed an innovative measurement approach using gamma-ray spectroscopy. Resolving the cross section from the experiments required a combined, intensive effort by experimentalists, nuclear theorists, and modelers. The new

Nonproliferation

Lasers



Energy & Environment

Biotechnology

Stockpile Stewardship

measurements promise a better understanding of the data collected from past nuclear tests, aiding current stockpile stewardship efforts.

The Laboratory's tradition in developing and using state-of-the-art accelerators has continued unabated since the early days. Livermore partnered with the Stanford Linear Accelerator Center and Lawrence Berkeley National Laboratory in the 1990s to build the 2.2-kilometer-circumference B Factory, which is elucidating the origin of the matter–antimatter asymmetry in the universe. (See *S&TR*, January/February 1997, pp. 4–13.) The team is now helping design the 25-kilometer-long teraelecronvolt Next Linear Collider to better analyze physics beyond the Standard Model. (See *S&TR*, April 2000, pp.12–16.)

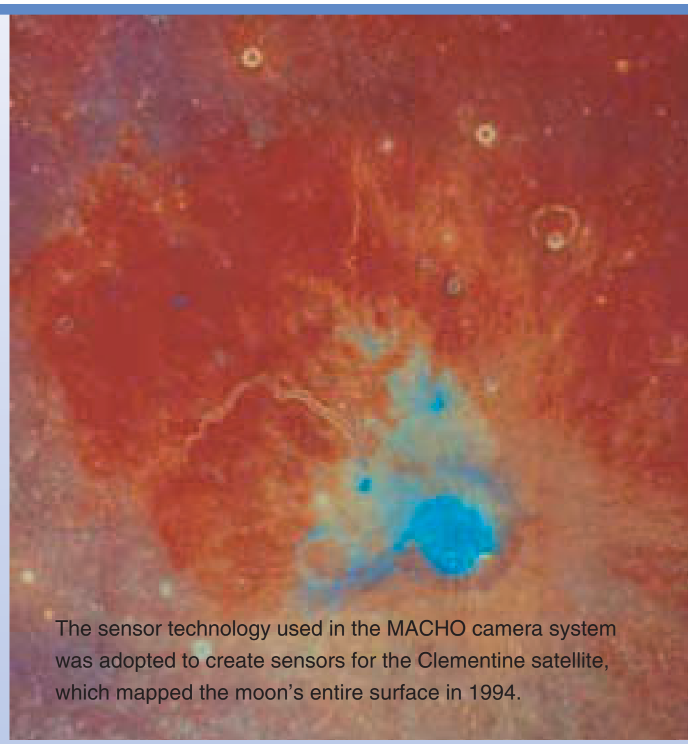
Divining the Heart of a Star

The same thermonuclear processes that drive a nuclear weapon drive the heart of a star. So, it's no surprise that astrophysics research at Livermore draws on the Laboratory's expertise in high-energy-density physics and complements the Laboratory's important stockpile stewardship responsibilities. In *Memoirs*, Edward Teller, who founded Livermore Laboratory along with E.O. Lawrence, notes, "From the beginning, and throughout the years to this date, Livermore has emphasized astrophysics and other branches of pure science in the recognition that great progress in applications cannot be made if science itself is neglected." In particular, Teller noted a paper by Stirling Colgate and Montgomery Johnson in 1960 that correctly described the mechanism and effects of an exploding star—a supernova. "The novelty in Montgomery and Stirling's work," explains Teller, "was their recognition that a shock wave, taking its origin in the center of the star and accelerating as it spread into the less dense regions of the star, was the first step in producing cosmic rays. That work is still cited as one of the more important papers in our current understanding of the universe." Research into astrophysics and general relativity continues, both at the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (see the box below) and within the PAT Directorate.

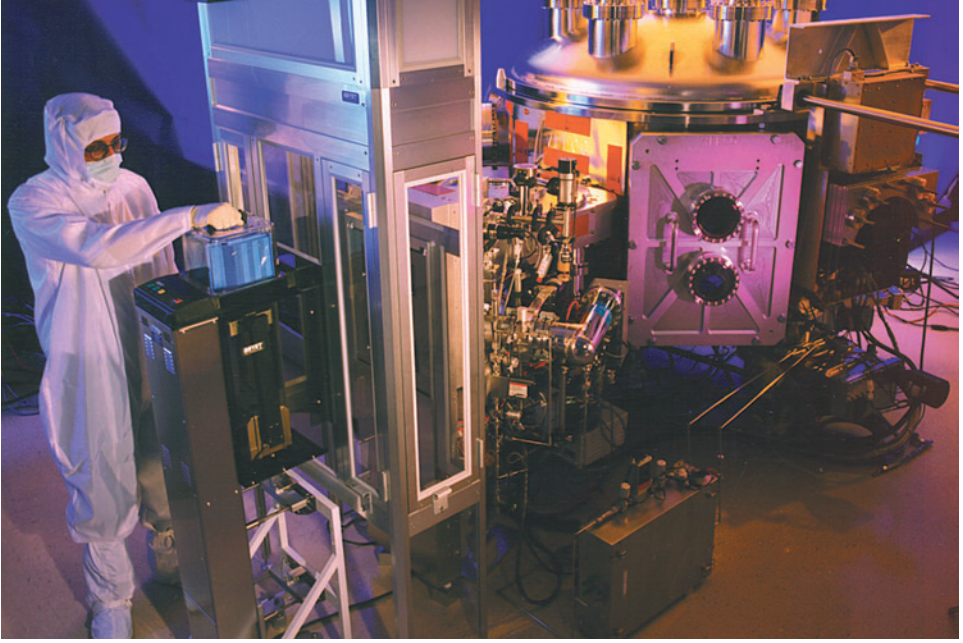
One example of current research applicable to astrophysics and stockpile stewardship is work on radiative opacity—that is, the study of how opaque a material is to the transport of photons. (See *S&TR*, April 1999, pp. 10–17.) Stellar opacity is concerned primarily with lighter elements, while opacity of nuclear weapon plasmas focuses on heavier elements; yet, the physics is similar for both. Researchers generally use detailed computer models to calculate opacities because it is extremely

Searching the Universe

One ongoing project of the Livermore branch of the University of California's Institute of Geophysics and Planetary Physics (IGPP) involves an attempt to identify the dark, invisible matter thought to comprise most of the universe's mass. (See *S&TR*, April 1996, pp. 6–11.) In the late 1980s, Livermore astrophysicist Charles Alcock, applying an innovative imaging technology invented for the Strategic Defense Initiative, searched for occasional amplifications of starlight from outside the galaxy caused by the gravitational effects of large objects known as MACHOs (massive compact halo objects). In 2000, Alcock, now a professor at the University of Pennsylvania, won the American Astronomical Society's Beatrice Tinsley Prize for his research. The data, which were collected by early 2000, are now being analyzed. They are also being used in another IGPP project to study the Milky Way's structure and composition. The IGPP is also home to the Djehuty project to develop a next-generation, fully three-dimensional, stellar structure and evolution code that will run on massively parallel computers. (See article beginning on p. 4.)



The sensor technology used in the MACHO camera system was adopted to create sensors for the Clementine satellite, which mapped the moon's entire surface in 1994.



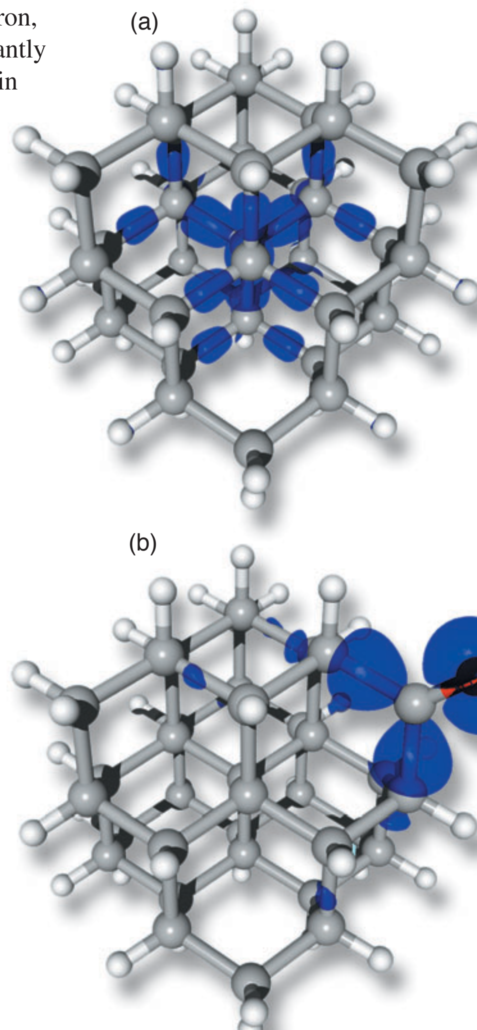
Livermore's early work on x-ray lasers and optics established technologies that led to its collaboration with industry and other national laboratories to develop extreme ultraviolet lithography for manufacturing the next generation of computer chips. Resulting microprocessors will be 100 times more powerful, and memory chips will be able to store 1,000 times more information than they do today. Livermore is the lead laboratory for optical design and fabrication, metrology, multilayer coating development, and mask fabrication for this project.

difficult to directly measure the opacity of materials hot enough to be in plasma form. In the early 1990s, physicists Forrest Rogers, Carlos Iglesias, and Brian Wilson built OPAL, a new model of stellar opacity that avoids many of the approximations and simplifying assumptions of earlier codes. In particular, OPAL accurately treats the myriad energy transitions in iron, which were previously overlooked in blocking radiation. OPAL calculations showed that iron, the most abundant heavy element in a star, can significantly impede radiation flow and therefore plays a major role in stellar properties. Throughout the 1990s, OPAL was refined through experiments on Livermore's Nova laser and on the Saturn pulsed-power machine at Sandia National Laboratories in Albuquerque. Data from these experiments and the codes they validate are being used to deepen astrophysicists' understanding of stars, strengthen fundamental knowledge of atomic processes in extreme environments, and provide greater confidence in the computational tools needed to maintain America's nuclear forces.

Creating Fusion in the Laboratory

It's little wonder that Herb York's original plan for the Laboratory included a group to research controlled thermonuclear reactions (CTR), or fusion energy. Not only are the physics processes of fusion similar to those of a nuclear weapon, but also interest in using fusion for power production was gaining ground in the early 1950s. The prospect was for a virtually inexhaustible, low-cost, safe, and environmentally attractive energy source.

The Laboratory initially concentrated on the magnetic confinement concept for producing fusion power, in which a magnetic force field traps a plasma long enough to achieve fusion. Livermore's approach was to use reflecting magnetic fields—or magnetic mirrors—to confine the fusion fuel. The first CTR group leader, physicist Dick Post, remembers, "In 1952, hardly anyone understood even the simplest aspects of the confinement of plasma by mirrors. There just wasn't any prior work to go on." Livermore physicists started with the basics, studying fundamental plasma processes; developing



Recent Livermore quantum molecular simulations examined the effects of contaminants such as oxygen on silicon quantum dots. A single oxygen atom can make a big difference on a quantum dot because of the dot's large ratio of surface area to volume. (a) In a simulation of a nanometer-size (71-atom) silicon quantum dot, the white hydrogen atoms bond to the surface, making the dot less reactive. The purple region, or "cloud," shows where light-absorbing electrons are most likely to be located inside the dot. (b) When two hydrogen atoms are replaced by an even more reactive oxygen atom, the electron charge cloud is drawn toward the oxygen atom, dramatically changing the optical properties of the

Sensors for Personal Health and the Health of the Nation

Innovative sensor and detector development for medical, national security, and defense-related applications is another focus of Livermore's physicists. In the Medical Technology Program, physicists, bioresearchers, and others are developing tools to provide cost-effective treatment for acute stroke, cancer detection and therapy, diabetes treatment and diagnostics, and therapy for other prevalent diseases of national importance.

For example, a microbead immunoassay dipstick system under development could be used by personnel such as firefighters and paramedics to run sophisticated diagnostics at the emergency site using a simple, one-step measurement. It could also be used as a portable clinical laboratory for military operations and for detection of biowarfare agents. Another tool, the Smart Probe, promises to provide early and accurate detection of breast cancer. The probe's sensors measure optical, electrical, and chemical properties that differ between healthy and cancerous tissues. Sensors play an important role in a program to develop an advanced interceptor for missile defense programs. The Advanced Technology Kill Vehicle uses lightweight integrated sensing systems to guide and control it while intercepting a missile. Cryogenic detectors, such as the one developed by physicist Simon Labov and his team, can distinguish between background radiation and nuclear materials and show promise in helping guard against the proliferation of nuclear weapons. (See *S&TR*, April 1998, pp. 16–18.)

methods to measure the temperature, density, and diffusion rates in a hot plasma; and exploring ways to contain the plasma.

Weapons and fission energy research also benefited fusion energy efforts, particularly in the search for reactor materials. John Anderson explains, "Fusion reactions produce large quantities of neutrons that can 'activate' the materials they hit, making the materials radioactive. You need to know how much radioactivity is generated, and you need accurate neutron transport models, topics of interest to weapons researchers as well." Beginning with the Table Top Reactor in 1954, Livermore created a series of machines to study the concept of plasma confinement using magnetic fields. More recently, Livermore fusion energy scientists are revisiting the spheromak concept of magnetic fusion. (See *S&TR*, December 1999, pp. 18–20.)

The tantalizing possibility of fusion energy took another turn with the invention of the laser in 1960. Some Livermore researchers, including physicist John Nuckolls (who later became a Laboratory director), wondered whether laser light might be able to trigger fusion reactions. Nuckolls and fellow physicists Ray Kidder and Stirling Colgate used Livermore-developed codes to study the possibility of compressing and igniting a small amount of deuterium–tritium fuel with powerful, short-duration laser pulses. These calculations revealed that to achieve energy gain—that is, to get more energy out than is put in—the laser would have to compress the fuel to about 1,000 times its liquid density.

In 1962, a small laser fusion project started in the Physics Department to explore this possibility. In the early 1970s, new computer calculations showed that interesting laser fusion experiments could be done with lasers as small as 10 kilojoules and that energy gains could be achieved with a megajoule-size laser. By this time, interest in laser fusion was widespread, and in 1972, the Inertial Confinement Fusion (ICF) Program was formed at the Laboratory. From this program sprung a series of increasingly powerful lasers, beginning in 1975 with Janus, a two-beam system with under 50 kilograms of laser glass, and leading to the National Ignition Facility, which will have 192 beams and over 180,000 kilograms of optics and is now under construction.

The x-ray laser also owes its existence to Livermore's early research into the physics of lasers. In the 1970s, physicists realized that laser beams could be generated by ions with high-lying energy states. In the 1980s, Livermore generated the first-ever x-ray laser beams in an underground test and demonstrated the first x-ray laser in a laboratory setting. In the 1990s, a Livermore team developed a small tabletop x-ray laser ideal for probing and imaging high-density plasmas. (See *S&TR*, September 1998, pp. 21–23.) These small x-ray lasers are used to fine-tune equations of state for a variety of materials, including those of interest to stockpile stewardship. Development of the x-ray laser also established the technical skills that helped lead to short-wavelength projection lithography for mass production of integrated circuits—a technology of significant importance to the nation's semiconductor industry. (See *S&TR*, November 1999, pp. 4–9.)

Understanding the World, Atom by Atom

"The preeminent goal of physics in the 20th century was to understand the workings of the world at the most fundamental level," says Goldstein. In the earlier part of the century, as physicists began studying atoms and their constituents, they learned that Newton's laws of motion did not apply on the small scale. The powerful mathematical tools of quantum mechanics were developed, and when computers arrived mid-century, with their geometric growth in computing power, physicists were in a better position to address the complexities of many particles interacting to produce the bulk properties of material systems.

At Livermore today, physicists such as Giulia Galli use the supercomputers of the Advanced Simulation and Computing (ASCI) program to simulate matter at a more fundamental level than was previously feasible. (See *S&TR*, April 2002, pp. 4–10.) Computer codes have been developed that allow researchers to simulate the interactions of 10 to 1,000 atoms and see in detail the dynamic activity of nanoparticles of individual atoms and molecules. For the silicon nanoparticles known as quantum dots, quantum simulations reveal unique optical properties that vary with size and surface characteristics. Lasers made of silicon are now possible, as are silicon dots that could be used as fluorescent markers in biological research and as biological sensors.

Growing Leaders and Programs

Throughout Livermore Laboratory's history, the physics organization has been the birthplace of new scientific concepts. It has grown programs that then split off to become their own considerable forces, provided inspiration and support for a recent Nobel Prize winner whose work was carried out at the Laboratory, and developed many of the Laboratory's top leaders. All but one of the Laboratory's directors were physicists, and many—including Edward Teller, John Nuckolls, and Bruce Tarter—at one time or another headed the physics organization. "From early on, Physics has provided top leaders to the Laboratory, and we've also played a role in providing new programmatic directions for the Lab," says Goldstein. "I see both roles continuing into the future in our work to keep the Laboratory at the scientific cutting edge."

—*Ann Parker*

Key Words: astrophysics, dark matter, fusion energy, nuclear cross section, opacity, quantum mechanics, sensors, stockpile stewardship, tabletop laser, thermonuclear processes, weapons research, x-ray laser.

For further information about the Physics and Advanced Technologies Directorate, see:
www-pat.llnl.gov/

For further information about the Laboratory's 50th anniversary celebrations, see:
www.llnl.gov/50th_anniv/

In December 1998, Robert B. Laughlin, a longtime Livermore employee and a professor of physics at Stanford University, received the 1998 Nobel Prize for physics for work he did in the Laboratory's condensed-matter division in 1983. The prize—shared with Horst Stormer of Columbia University and Daniel Tsui of Princeton University—was awarded for the discovery that electrons acting together in strong magnetic fields can form new types of particles with charges that are fractions of electron charges. (See *S&TR,* January/February 1999, pp. 15–18.)

Photo: AP/Jonas Ekstromer

The Outlook Is for Warming, with Measurable Local Effects

Our planet's climate is warming up. The effects are, for the first time, visible on a regional scale.

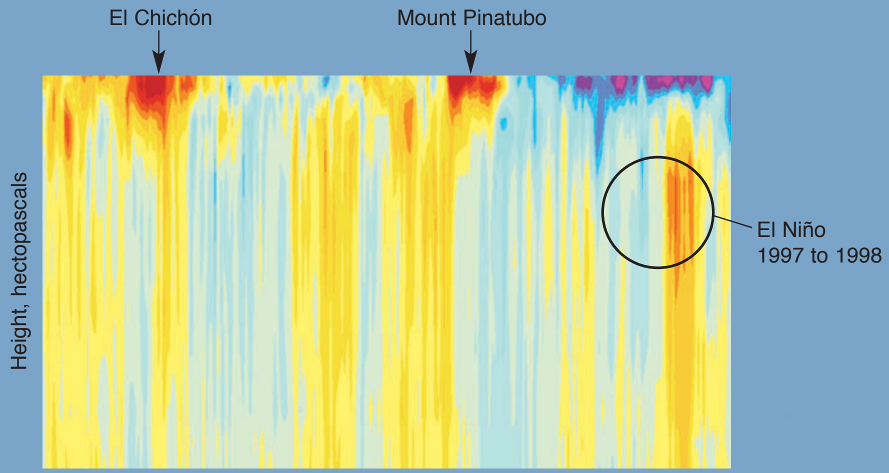
GLOBAL warming. Few phrases elicit so much controversy today. But is our climate truly changing? And if it is, do we know why it is changing?

At the United Nations, the Intergovernmental Panel on Climate Change (IPCC) certainly thinks the world is getting warmer and puts much of the blame on human activity. In its 2001 *Third Assessment Report*, the IPCC projects that average global temperature will increase by 1.6° to 6°C by 2100.

The report indicates that, globally, the 1990s were the warmest decade on record, with 1998 the single warmest year. Accompanying this global-scale temperature increase were changes in other climate variables, such as precipitation, snow cover, glacier extent, and sea level. The changes in these variables are broadly consistent with the IPCC's estimate that Earth's surface warmed by roughly 0.6°C over the 20th century. The 2001 IPCC report concluded that "there is new and stronger evidence that most of the warming observed over the last 50 years is attributable to human activity."

Atmospheric carbon dioxide and other trace gases help keep our planet warm by absorbing some of the Sun's heat that the Earth would otherwise emit back into space. This natural greenhouse effect makes Earth's surface about 34°C warmer than it would be without greenhouse gases. But human activities, such as the burning of fossil fuels, have added greenhouse gases to the atmosphere. Atmospheric carbon dioxide levels, for example, have increased by about 30 percent since the beginning of the Industrial Revolution. This human-caused enhancement of the natural greenhouse effect has contributed to the warming of the planet over the last century.

Climate change can occur even in the absence of human activities. The climate system is like a bell that rings in a certain way. One form of "ringing" is



Globally averaged temperatures have changed at different levels in Earth's atmosphere. This profile is from close to Earth's surface through to the stratosphere. Temperatures are in the form of departures (anomalies) from long-term monthly means computed from 1979 to 1999 and are in degrees Celsius. The stratospheric warming caused by the El Chichón and Mount Pinatubo volcanic eruptions is clearly evident, as is the cooling of the lower atmosphere after Pinatubo. Results are from the so-called reanalysis project jointly performed by the National Center for Environmental Prediction and the National Center for Atmospheric Research.

the ocean warming phenomenon known as El Niño or its cooling sister, La Niña. Such changes are thought to be due to the internal variability of the climate system. But external events can also cause natural climate changes. Large volcanic eruptions can pump massive quantities of dust into the upper atmosphere (the stratosphere). The dust may remain in the stratosphere for years, cooling Earth's surface by absorbing and reflecting some of the incoming sunlight. Natural changes in the Sun's energy output and slow changes in Earth's orbit can also influence climate.

Carbon dioxide and other greenhouse gases get the most press, but there are other human influences as well. Changes in land use can be a concern. For example, Livermore scientists recently showed that human-caused changes in land-use patterns (especially conversion of forests to farm land) may have caused a gradual global cooling of approximately 0.25°C, mostly before the 20th century.

Large-scale burning of rain forests sends particulate matter into the lower atmosphere, warming us. At the same time, with fewer trees, less carbon dioxide can be absorbed from the atmosphere, which warms us further. Land surface changes also affect Earth's reflectivity, or albedo.

If Earth is getting warmer, is it possible to expose individual factors causing climate change? And what will global warming mean on a regional level? Two Livermore research teams are searching for—and finding—answers.

Atmospheric scientist Ben Santer, a 1998 John A. and Catherine T. MacArthur Foundation Fellow, has used sophisticated climate models to separate the effects of recent major volcanic eruptions and El Niños from other causes of climate change. The motivation for this research was to shed light on one of the outstanding puzzles in climate science: why Earth's surface has apparently warmed faster than the lower atmosphere.

At the same time, a team led by physicist Philip Duffy has brought the highest resolution yet to global climate modeling, revealing a wealth of regional effects for the first time. Instead of a 300-kilometer grid—the previous state of the art—Duffy's team has been able to perform global simulations using models with grid cell sizes of 75 and even 50 kilometers. These are the finest-resolution global climate simulations performed to date. The figure on p. 6 compares these resolutions.

Duffy's work would not be possible without Livermore's massively parallel supercomputers, which can quickly perform the computationally demanding calculations inherent in global climate modeling. The first simulations using the 50-kilometer grid ran on the Advanced Simulation and Computing (ASCI) White computer during its initial, unclassified testing period in December 2000. Because the ASCI White computer is now used exclusively for classified computations, models used by Duffy's group are being run on other supercomputers at Livermore and at Lawrence Berkeley National Laboratory.

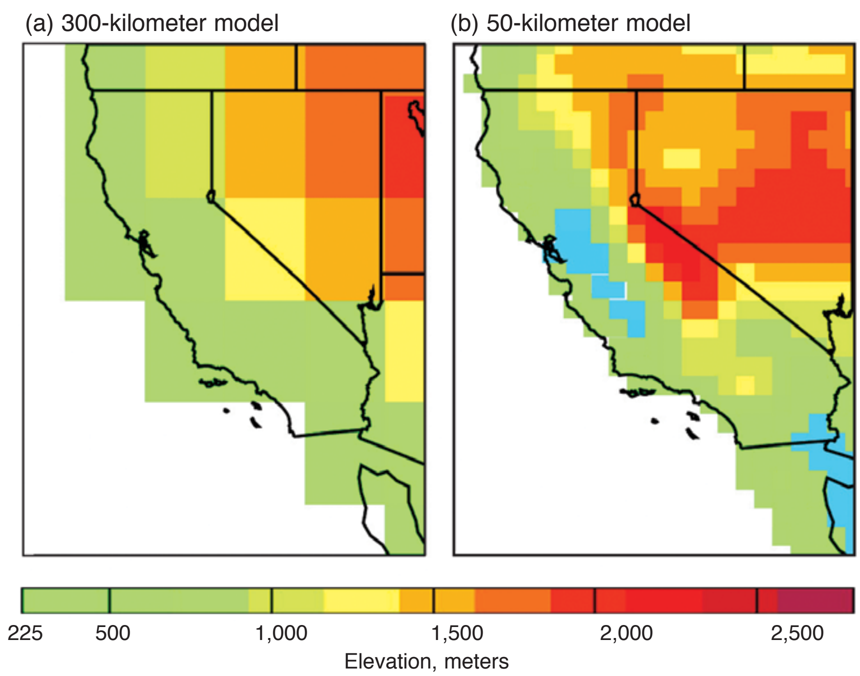
A 1-year simulation of global climate using the 300-kilometer grid can now be accomplished in 4 or 5 hours. Five years ago, it would have taken over a day to complete a comparable simulation. For the 50-kilometer grid, "At best, we can do about a month of simulated climate in a day," says Duffy. A 50-kilometer grid for climate modeling was the stuff of dreams 5 years ago.

Why the Controversy?

Much of the controversy about global warming results from two apparent contradictions. One relates to observed temperature data and the other to the issue of how well computer models of the global climate system can represent such observations.

While Earth's surface has warmed by about 0.15° to 0.2°C per decade since 1979, temperatures in the troposphere (the layer of the atmosphere extending from Earth's surface to 8 to 16 kilometers above it) have shown little warming, and even a slight cooling.

The apparent lack of tropospheric warming from 1979 to the present has been used to cast doubt on the reality of strong surface warming. It is important to understand whether this difference between surface and tropospheric warming rates is real or is an artifact of data problems. If this difference is real, what factors might be causing it?



The topography of California and Nevada is simulated in models with (a) 300-kilometer and (b) 50-kilometer grids. Models that use the 300-kilometer grid have been the state of the art, but Livermore has developed a 50-kilometer-grid model. Even with 50-kilometer grids, the topography of California and Nevada is not represented. The Coast Range mountains are not visible in (b), and the data smoothing process lowers the elevation of the Sierra Nevada mountains.

The second puzzle relates to the inability of many climate models to simulate the apparent difference in surface and tropospheric warming rates. This inconsistency is sometimes used to bolster arguments that models are inappropriate tools for making projections of future climate change.

Recent work by Santer and his colleagues has addressed both of these puzzles. They have learned that at least some of the differential warming of Earth's surface and lower troposphere is real and attributable to the combined effects of stratospheric ozone depletion, volcanic eruptions, and natural climate variability. Differences in the geographic regions sampled by the surface thermometer network and the satellite-based tropospheric temperature measurements also explain some of the divergent temperature changes of the surface and troposphere.

"But," Santer concedes, "accounting for these effects still does not fully explain the different rates of temperature change. Nor does it explain why models don't reproduce this differential behavior accurately."

A Search for Resolution

For several years, Santer has been working with other investigators at Livermore and research institutions around the world to reconcile the apparent contradictions in actual data and global climate models. In one study of climate between 1979 and 1998, they discovered that a model including anthropogenic (human-caused) factors and volcanic aerosols produced surface–troposphere temperature differences that were the closest yet to actual observed data.

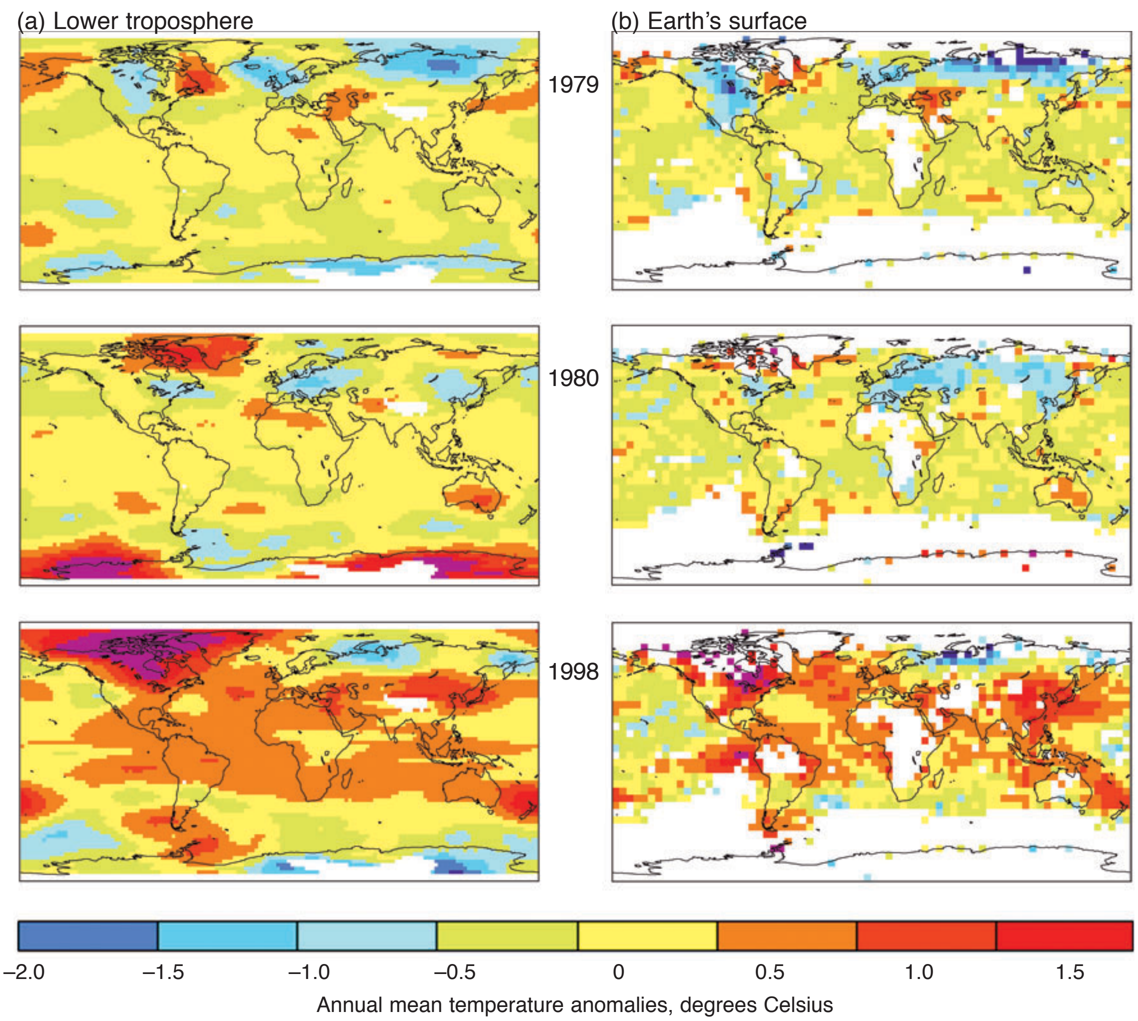
As a follow-up, they wanted to examine the influence of volcanoes alone. But, says Santer, "We had a bit of bad luck. Nature made our lives difficult. There was a major El Niño in

1982, at the same time as the eruption of El Chichón in Mexico. A smaller El Niño coincided with the 1991 eruption of Mount Pinatubo in the Philippines. This made it tough to disentangle the effects that volcanoes and El Niños had on surface and tropospheric temperatures."

Santer and his Livermore colleagues had been doing similar work for the past 10 years. For the first half of that time, they were trying to identify human-caused climate signals in observed temperature records. This involved using both model and observational climate data to understand the characteristic fingerprints of the many natural and anthropogenic influences on climate. (See the figure on p. 8.)

Previous researchers had attempted to remove the effects of explosive volcanic eruptions and El Niños from surface and tropospheric temperatures so they could obtain better estimates of the underlying human component of climate change. But Santer's team was the first to deal fully with the correlation of volcanic eruptions and El Niños, known in statistical problems as collinearity.

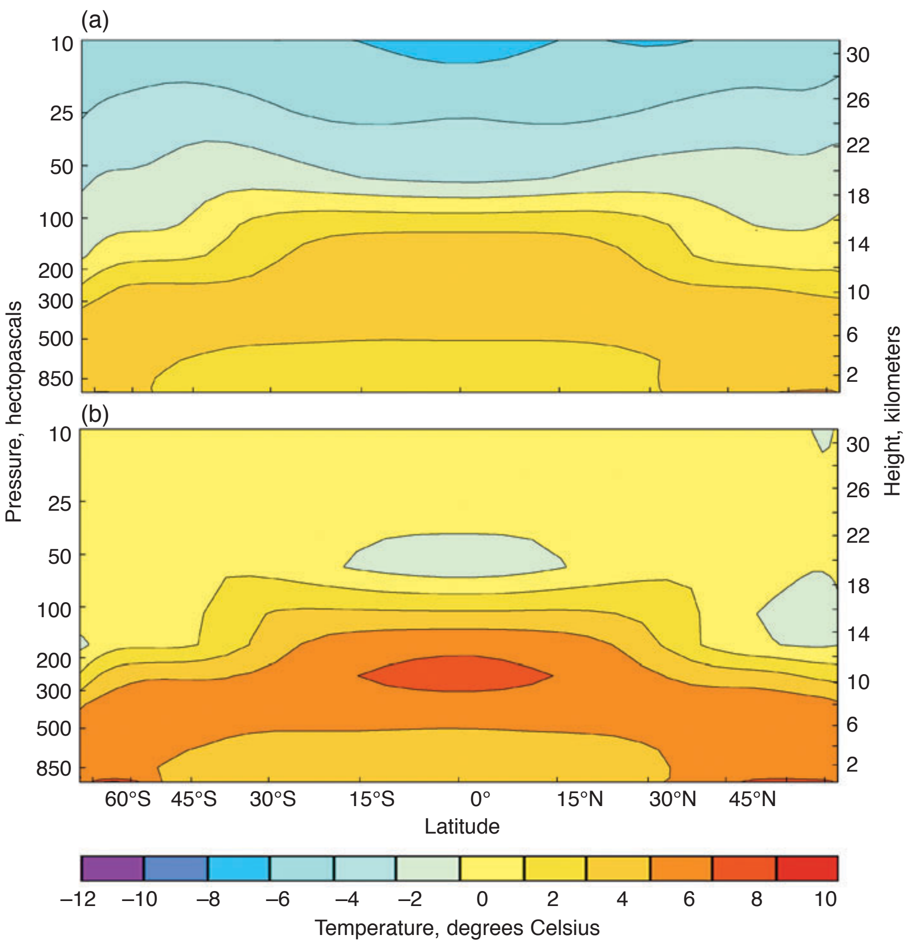
The team's observational data were land and ocean surface temperatures compiled at the Climatic Research Unit in Norwich, England, together with satellite-based tropospheric temperature measurements. Their model data came from a number of different sources: the Max Planck Institute for Meteorology in Hamburg, Germany, the Goddard Institute for Space Studies in New York, and the National Center for Atmospheric Research in Boulder, Colorado. Researchers from all of these organizations participated in the team. Other team members were with Livermore's Program for Climate Model Diagnosis and Intercomparison,



Geographic patterns of annually averaged temperature anomalies in (a) the lower troposphere and (b) at Earth's surface. Tropospheric temperature measurements are from polar-orbiting satellites, and surface measurements were made by thermometers. White areas denote missing data. Although the satellites have near-global coverage, the surface data have large gaps. Comparing satellite and surface data over areas of common coverage helps to explain some of the differential warming of the surface and troposphere. Anomalies are expressed relative to annual mean temperatures averaged over 1979 to 1998.

which routinely develops methods and tools for the diagnosis, validation, and intercomparison of global climate models.

The team first dealt with observed data. They found that removing El Niño and volcanic effects always led to larger warming trends in the residual surface and lower tropospheric data than in the raw observational data (where these effects were left in). Although El Niños caused a small net warming from 1979 to 1999, the El Chichón and Mount Pinatubo volcanic eruptions caused a larger net cooling during the same period. Removing both El Niños and volcanoes more clearly revealed the underlying warming trend in surface and tropospheric temperatures. It also helped to explain some of the differential warming of the surface and troposphere.



(a) Atmospheric temperature changes predicted to occur in response to a doubling of preindustrial levels of carbon dioxide. (b) Projected temperature response to a 2-percent increase in the Sun's energy output. Each factor that influences our climate has a characteristic "fingerprint." Scientists typically use computer models of the climate system to gain information on these fingerprints. In a model, it is possible to study the climatic effects of a single influence only, such as changes in atmospheric carbon dioxide. This is not feasible in the real world, where multiple factors that influence climate are changing simultaneously. Both (a) and (b), which are clearly dissimilar, show annual mean changes (in degrees Celsius) as a function of latitude and altitude.

"It's clear that if the Mount Pinatubo and El Chichón eruptions had not occurred, the lower troposphere would have experienced more pronounced warming," says Santer.

The team then removed volcanic and El Niño effects from model output and compared the results with observations. It is important to do this because even in a model with "perfect" representation of El Niño variability, the simulated El Niños would not necessarily occur at the same time that they happened in the real world. Also, some model experiments include the effects of well-observed volcanoes (such as Mount Pinatubo) but exclude other eruptions where less is known about the properties of the volcanic aerosols. Removing volcano and El Niño effects from both models and observations allows a fairer comparison of the underlying simulated and observed responses to human-caused changes in greenhouse gases.

The general conclusion from such comparisons was that removing volcano and El Niño effects from atmospheric temperature data improves the correspondence of the modeled and observed differential warming of the surface and troposphere over the last several decades. It does not, however, fully reconcile models and reality. The remaining differences are probably caused by problems with the observational temperature data; missing or inaccurately specified "forcings" in the climate model experiments, such as the neglect of land use changes or aerosol particles from biomass burning; and errors in the climate responses that the models predict.

Santer and his colleagues are actively investigating these possibilities. "We hope we've showed that this is a complex scientific issue," says Santer. "It can't be reduced to a one-minute sound bite. This issue is important, because it relates to our ability to evaluate climate models and to determine whether these models are useful tools for predicting climate change over the next century."

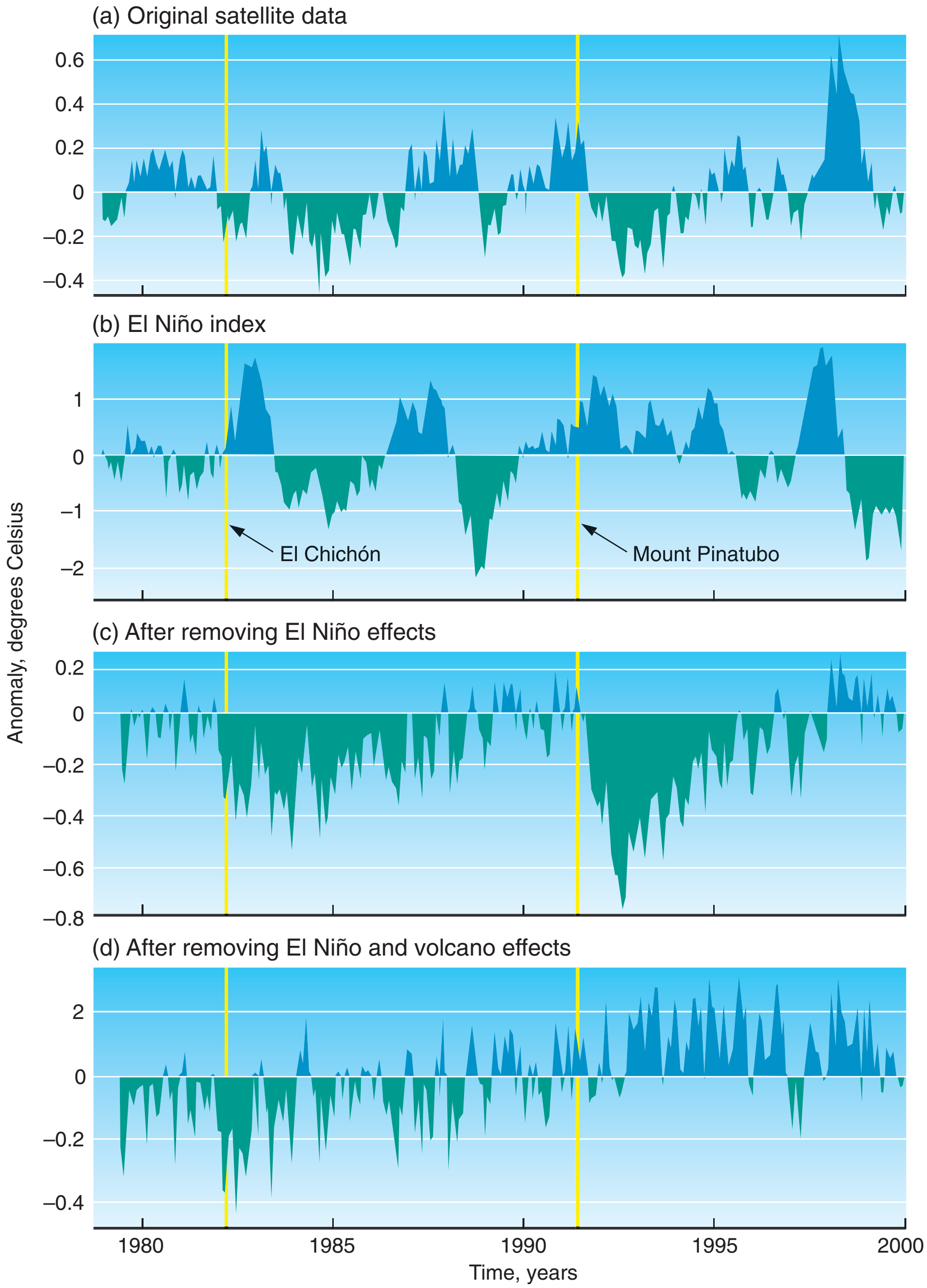
An Up-Close Look

The IPCC's prediction that mean global temperatures will increase from 1.6° to 6°C by the end of this century isn't especially useful for farmers and others whose livelihoods depend on the weather. They need more specific information on temperature increases expected in their area, whether it be Kansas or Kenya. They also need to know about changes in temperature extremes and in other important quantities such as precipitation. By providing improved simulations of climate change on regional scales, Livermore's high-resolution climate simulations should allow for more accurate assessments of the effects of climate change on society.

Grids of 50 kilometers and less are already used in numerical weather prediction, which is much less computationally intensive than climate modeling because it requires much shorter forecasts (days rather than decades). For long-term climate modeling with resolution this fine, scientists had to await the arrival of huge computers with hundreds of processors operating simultaneously.

Duffy's team is using the Community Climate Model 3, or CCM3, an atmospheric model developed by the National Center for Atmospheric Research (NCAR) in Boulder, Colorado. CCM3, the fourth-generation CCM model, is used at coarse resolutions in climate modeling centers around the world.

"For every change in horizontal resolution, there's the problem of retuning the model," says Duffy. Several physical processes such as convection, cloudiness, and precipitation are too small to be represented explicitly in climate models and are therefore treated using semiempirical parameterizations.



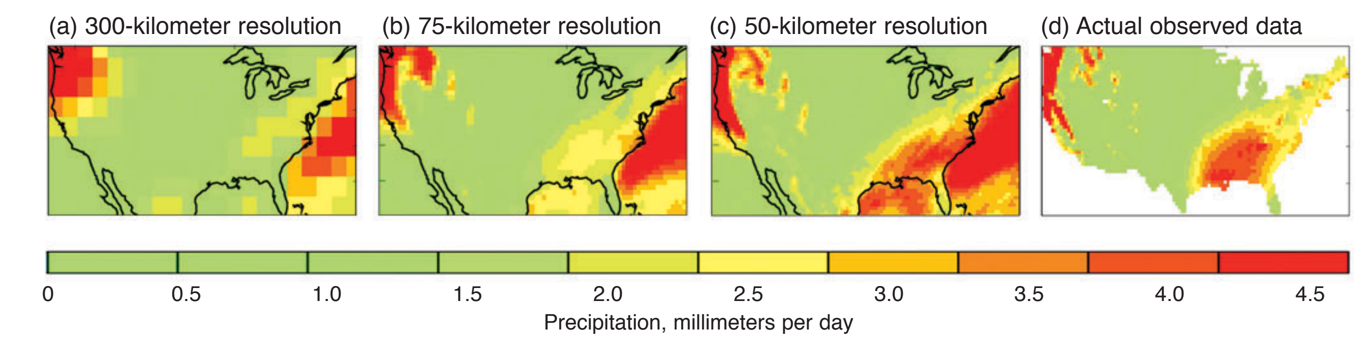
Some of the problems involved in removing the effects of El Niño variability and explosive volcanic eruptions from tropospheric temperature data. (a) In the original satellite-based temperature data, the cooling signal of the 1983 El Chichón eruption is masked by (b) one of the strongest El Niño events of the 20th century. After using an iterative method to successively refine estimates of El Niño and La Niña effects on tropospheric temperatures, these effects are removed from the original temperature data in (a). The cooling effects of the El Chichón and Mount Pinatubo eruptions are now more easily seen in (c). It is clear in (d) that removing both volcanoes and El Niño effects yields a pronounced warming trend that was not apparent in the original temperature data.

For example, although clouds may be too small to be represented directly in a grid cell, they must be accounted for because cloud cover affects the flow of radiation in the atmosphere. "So we parameterize their effects by modifying the optical properties of that layer of the atmosphere," says Duffy.

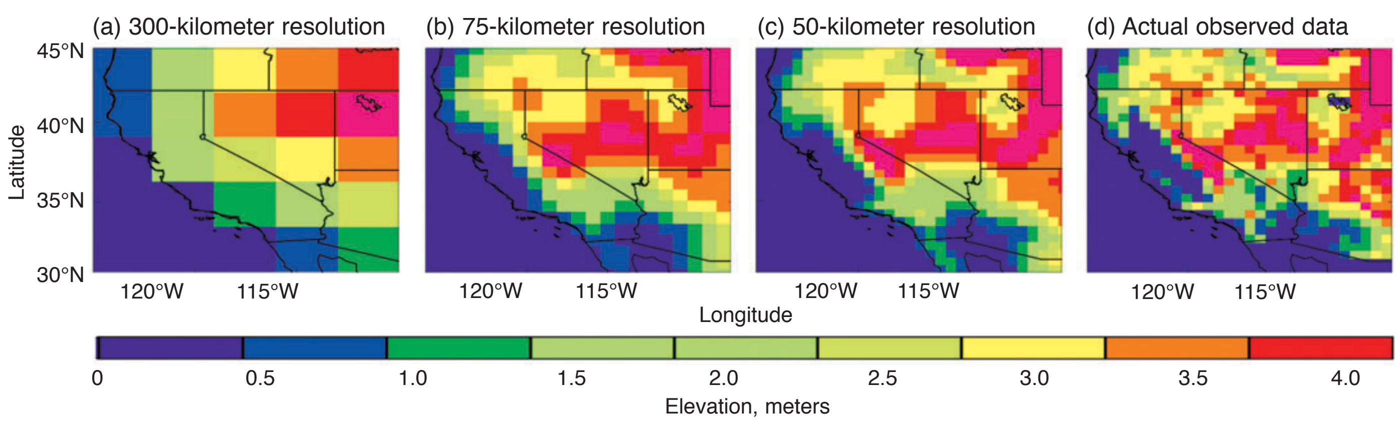
Because these parameterizations are not based on first-principles physics, they must be tuned carefully at each resolution. Tuning is done by adjusting parameter values to make the model's results agree as closely as possible with observations. The 300-kilometer model has already been carefully tuned at NCAR to optimize results at that resolution. In collaboration with researchers at NCAR, Livermore researchers retuned their 75-kilometer model. Thus far, tuning done for the 75-kilometer model has also worked reasonably well with the 50-kilometer grid.

The team's proof of principle with the 50- and 75-kilometer models was to compare their modeling results to observed data. Although, as Duffy notes, "the 50-kilometer model actually has better resolution than most of our observational data." Perhaps not surprisingly, simulations using the 50-kilometer model agreed better with observed data than either a 75- or 300-kilometer grid. In some cases, there were substantial improvements.

When the team examined results in more localized regions of interest, the results were striking. The upper figure below shows simulated precipitation over the U.S. in December, January, and February using 50-, 75-, and 300-kilometer grids and compares all three to observed data. As the grid size shrinks, both small-scale and large-scale simulated precipitation features converge toward observations. This example shows



The representation of December, January, and February precipitation over the U.S. improves as the resolution increases. Simulations using (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution are compared with (d) actual observed data. Both fine- and large-scale aspects of the simulation improve as spatial resolution shrinks.



A comparison of elevations in California, as represented in models having (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution, with (d) actual elevations at 50-kilometer resolution. Elevations in the models are lightly smoothed—evened out—to prevent sudden changes that cause numerical noise and contaminate the results. Even at 50-kilometer resolution, California's Coast Range mountains and the Central Valley are not well represented.

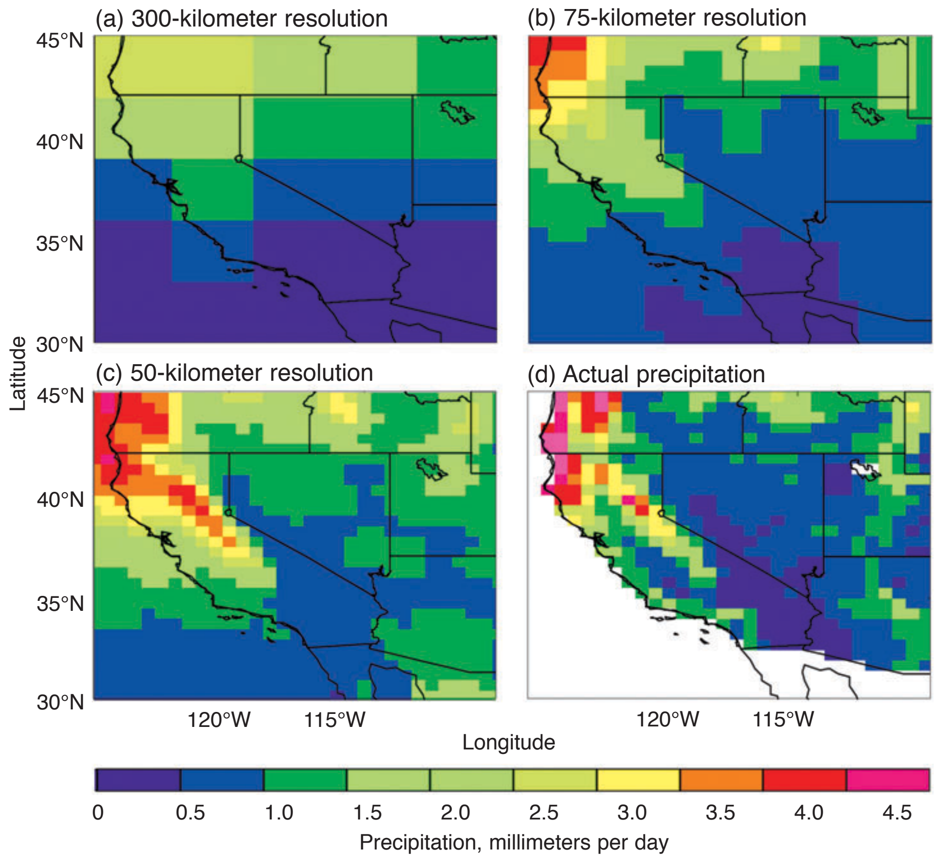
that as spatial resolution becomes finer, not only is fine-scale detail added to the model results, but the large-scale aspects of the solution also become more realistic.

Simulations of California climate are a real test of climate models because of the great variability in climate that occurs within the state's relatively small area. Much of this variability results directly or indirectly from the state's major topographic features: the Coast Range, the Central Valley, and the Sierra Nevada. The figure at left, bottom, compares actual elevations at 50-kilometer resolution with topography as represented in models having 300-, 75-, and 50-kilometer resolutions. Although the topography is more realistic as the model resolution becomes finer, neither the coastal mountains nor the Central Valley are adequately represented in even the 50-kilometer model.

In part because of improved representations of topography, the model's ability to simulate precipitation in California improves dramatically as the resolution becomes finer. Nonetheless, 50-kilometer resolution is still not adequate to represent the state's Coast Range and Central Valley; even at this resolution, the simulation of precipitation differs noticeably from observations.

Simulations of Arctic climate similarly improve dramatically with finer resolution, but further improvements are nonetheless needed. Most coarse-resolution ocean–atmosphere–sea ice climate models produce poor simulations of the pattern of sea-level pressure in the Arctic region. Poor data for sea-level pressure result in unrealistic simulated atmospheric circulation, which in turn produces unrealistic distributions of sea ice thickness and concentrations and other problems. Accurate predictions of sea ice and of changes in sea ice because of global warming are essential. Sea ice strongly affects the climate not only in polar regions but also in far-flung regions through influences on the large-scale ocean circulation and on Earth's radiation balance.

In addition to these simulations of the present climate, Duffy's team has simulated the effects of increased greenhouse gases (that is, global warming) with the 75-kilometer-resolution model. This is the finest-resolution simulation of global warming performed to date and shows very different results from comparable simulations performed at coarser resolutions. Although the globally averaged responses of temperature and other variables to increased greenhouse gases are quite similar in the 75-kilometer model and in coarser-resolution models, the regional responses can be very different. For example, the figure on p. 12 shows predicted wintertime temperature changes between 2000 and 2100 in the U.S. The finer-resolution model shows regions of strong warming in the western U.S. and southeastern Canada, which are not predicted by the coarser-resolution model. In at least some cases, it seems clear that the results of the finer-resolution model are more believable.



A comparison of precipitation over California, as represented in models at (a) 300-kilometer, (b) 75-kilometer, and (c) 50-kilometer resolution, with (d) actual precipitation at 50-kilometer resolution.

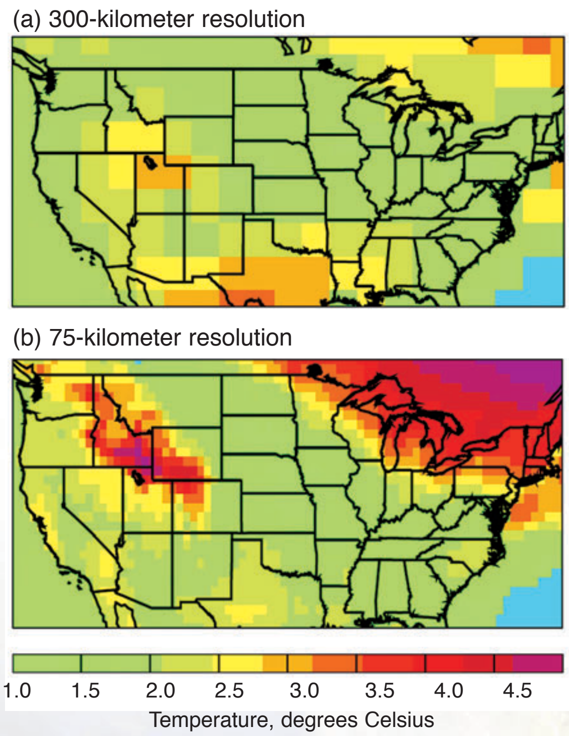
Duffy's group has already fielded inquiries from experts interested in the effects of localized climate change on crop diseases, human health, water resources, and the like. Although the finer-resolution models are far from perfect, they may represent the best tools available today for assessing the regional effects of global warming.

Getting It Right

A few months ago, a chunk of ice larger than Rhode Island collapsed on the east side of Antarctica. It was the largest single event in a series of ice shelf retreats there extending back 30 years. Temperatures at the Antarctic Peninsula have increased by 2.5°C over the last 50 years, much faster than the global average. Getting Arctic and Antarctic models right is crucial for determining what may happen to sea levels around the world as temperatures continue to rise.

Closing in on how much humans are responsible for the changes in our planet's climate is equally important. Getting it right matters to us all.

—*Katie Walter*



Predicted temperature increases from 2000 to 2100 for December, January, and February at resolutions of (a) 300 kilometers and (b) 75 kilometers. The predicted data from the model with finer resolution are much more specific and useful.

Key Words: climate modeling, Community Climate Model 3 (CCM3), global warming, National Center for Atmospheric Research (NCAR).

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For information about the Intergovernmental Panel on Climate Change:
www.ipcc.ch/

For information about Livermore's Program for Climate Model Diagnosis and Intercomparison:
www-pcmdi.llnl.gov/

Converting Data to Decisions

ENVIRONMENTAL data aren't easy to obtain, and once obtained, they are often hard to interpret. For example, drilling into the earth to determine what kind of soil exists at any given spot in the substrate is not only expensive but also gives scientists just piecemeal information. Computer analysis with this information can be equally piecemeal. But earth scientists are learning that computer models can be made more meaningful when they are stochastic, meaning that they are based on a certain amount of probability. Now, with the capability of high-performance supercomputers in the National Nuclear Security Administration's Advanced Simulation and Computing (ASCI) program, Livermore scientists are exploring groundbreaking ideas in statistical theory that will help them use stochastic descriptions quantitatively and obtain a much more complete picture of soil composition.

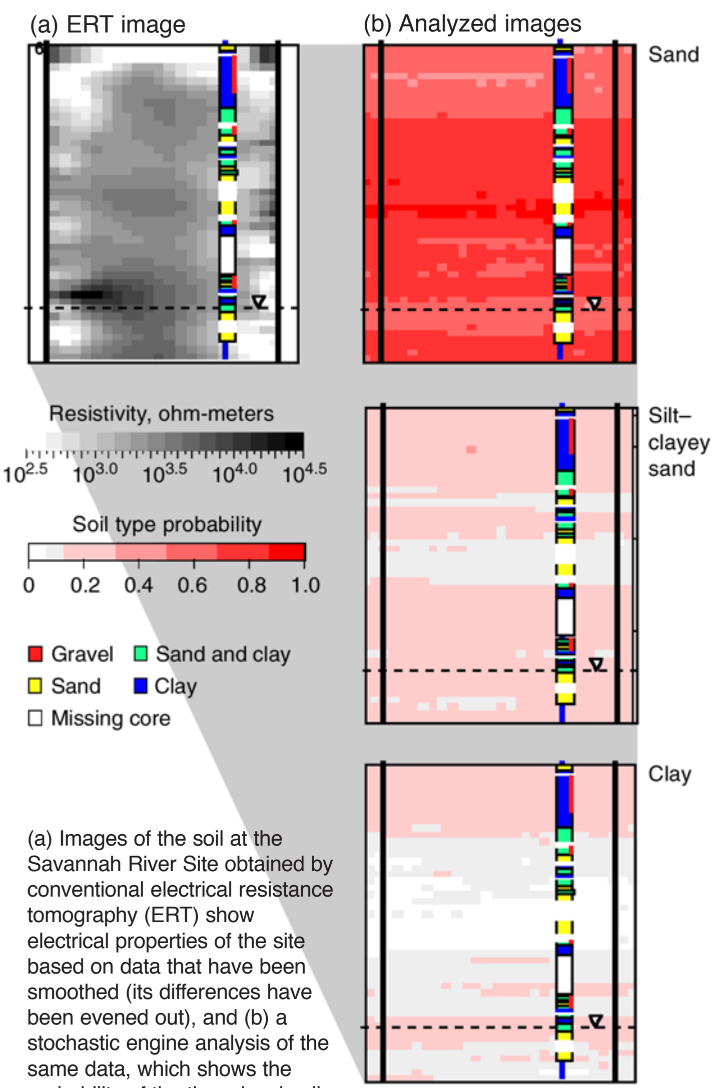
This new technology, called a stochastic engine, is a process that links predictive models, advanced statistical methods, and refined search methods. Using this technology, scientists can incorporate a proposed soil configuration into a computer model and produce a geophysical simulation. The simulated result is compared to actual data. If the result is consistent with observed data, then the simulation is boosted to the next phase of analysis.

The stochastic method is a powerful technique that is now in use. Livermore scientists are consulting on a project with the Westinghouse Savannah River Company in which the stochastic engine will assist in a major cleanup operation at the Savannah River Site in South Carolina. The method could also be applied to problems in stockpile stewardship, atmospheric dispersion, seismic velocities, and intelligence collection.

Cleanup Site Yields New Tool

The stochastic engine concept uses techniques developed at Livermore and was motivated by an innovative steam remediation cleanup being conducted by Southern California Edison at a Superfund site in Visalia, California, in which Laboratory scientists also participated. (See *S&TR*, January/February 1996, pp. 6–15.) During the course of the project, more than 46 million pieces of data were obtained pertaining to the way steam, water, and contaminant flowed through the groundwater plumbing system. These data included temperatures, flow rates, pressures, and electrical resistance tomography (ERT) measurements. ERT, a

technology developed at Livermore in 1993 and now available commercially, is similar to a computed tomography scan. It images soil resistivity, and that gives scientists information on soil properties such as temperature, soil type, and saturation. While the data collected from Visalia were rich and invaluable for Edison's operational decisions, the various data types could only be used independently. Observations and simulations could not be linked to provide the kind of cohesive understanding that would dramatically improve site operations and, most importantly, optimize the final outcome of the cleanup work.



(a) Images of the soil at the Savannah River Site obtained by conventional electrical resistance tomography (ERT) show electrical properties of the site based on data that have been smoothed (its differences have been evened out), and (b) a stochastic engine analysis of the same data, which shows the probability of the three local soil types (sand, silt–clayey sand, and clay) at each location.

The work at Visalia, while highly successful overall, is representative of a frustration that Livermore environmental scientists experience whenever they attempt to characterize soil compositions at cleanup sites: how to apply the powerful predictive capabilities of Livermore's supercomputers to complex, real situations. For the past year, Roger Aines and a multidisciplinary team have been discussing how to apply modern computational power and statistical search methods to extract maximum information from sparse initial data and then to improve the analysis on the fly as more data become available.

More Than One Right Answer

The power of the stochastic engine comes from its ability to refine a model by successively narrowing down the possible configurations of a hypothetical model. The refinement is done over progressive layers of data. In this process of model improvement through iteration, the stochastic engine uses an advanced statistical method called a hybrid Markov Chain Monte Carlo (MCMC)–Bayesian analysis. In the MCMC analysis, a chain (or sequence) of configurations is considered. Each configuration undergoes a probability calculation that compares observed data to corresponding model predictions. If the predictions are acceptable (that is, probable for the configuration), the result of that calculation becomes the basis of the next configuration. This allows the process to rapidly search for good configurations in very complex situations. The Bayesian statistical method, based on the work of English mathematician Thomas Bayes, performs its part in the stochastic engine by comparing the probability calculations with real information to guide the statistical inference process.

Suppose a volume of soil is known to be composed of seven layers that could be either sand or silt, and an ERT measurement of that volume gives a value of 11. The stochastic approach calculates which configurations of silt and sand, and in which positions, give values close to 11. Each case with a value near 11 is passed on to the next stage of analysis. There, the model will continue to restrict possible configurations but base its decisions on other data types, such as water, temperature, or pressure.

For the simple case cited here, it is easy to calculate and compare all the possible configurations, but for a large area, such as the Visalia cleanup site, the possibilities are far too numerous. At Visalia, the MCMC–Bayesian method could help by performing an efficient intelligent search through the collection of possible soil configurations, rapidly identifying the configurations that most closely match all the data.

"It's not about trying to find the single best answer, but all of the good answers," says Aines. "In underground problems, there are usually multiple solutions that are consistent with the data."

The stochastic engine's ability to choose system configurations that are consistent with observed data allows much more tightly constrained (better restricted) answers than conventional methods. Only the ways the system can possibly exist are considered. Using the stochastic technique, for example, ERT images can be interpreted to derive characteristic soil types for a site, rather than simply provide the electrical properties of the ground. The stochastic engine allows the available information to be used more effectively. It also allows the user to incorporate known constraints, such as the presence of a gravel layer observed in a well, to further guide the statistical inference.

It Doesn't Have to End with Dirt

The stochastic engine method has tremendous potential for use in disciplines that need to combine data and simulation. Currently, the team is working with a number of scientists from other Livermore directorates to put the method to use, to identify unknown sources of toxic contaminants in the atmosphere, locate flaws in buildings, evaluate intelligence data, and expand tomography and x-ray imaging data.

The Savannah River Site project illustrates how the engine is being used in industrial partnerships. Livermore has been consulting with Westinghouse's Savannah River Company to clean up organic solvents from the soils and groundwater at the South Carolina site. Since 1983, the company has been performing environmental cleanup of a site where, over time, solvents became a solvent plume that extended over 5 square kilometers. Now, Westinghouse is ready to present its cleanup results to regulators and assure the community that the remaining plume will not affect surface water bodies. The stochastic engine will be used to evaluate the effectiveness of source cleanup and to predict the ultimate effect of the remaining plume.

Challenges Ahead

Why hasn't the stochastic method been used before? For one thing, the complexity of the method has required robust computer power that simply has not been available until recently. For another, even with the power available with ASCI computers, some are still skeptical of the method. Because underground problems are so complex, Aines says that many people are displaying a "show me first" attitude toward the technology. "No one has done this before, so some believe it can't be done." The Savannah River Site project may prove that the engine is a feasible and valuable tool for environmental cleanup and more.

—Laurie Powers

Key Words: Bayesian statistics, electrical resistance tomography, Monte Carlo method, Savannah River site, stochastic engine, Superfund, Visalia cleanup.

For further information contact Roger Aines (925) 423-7184 (aines1@llnl.gov).

Steve Carlat the A/M outfall site and (inset)examining the soil in a streamcut just below the outfall, looking at the silt layers that tend to control the migration of solvent that soaked into the soil from the sewer.

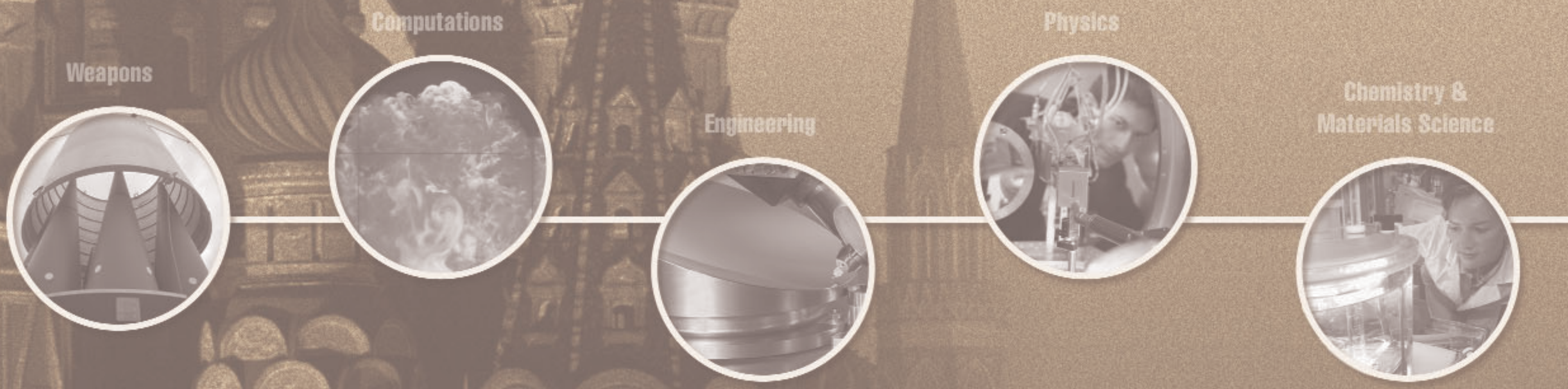
Knowing the Enemy, Anticipating the Threat

In a way, Lawrence Livermore was founded as a result of the nation's not knowing—or at least, underestimating—"the enemy." In August 1949, U.S. reconnaissance planes detected radioactive debris near Japan, proof that the Soviets had detonated an atomic bomb. In *Memoirs*, physicist Edward Teller writes, "Until the fall of 1949, our intelligence community, most of the leading scientists, and general public opinion held that the Soviet Union could not develop an atomic bomb before the 1960s." Within days, Ernest O. Lawrence, Nobel laureate and head of the University of California's Radiation Laboratory, met with federal officials to press for a strong hydrogen bomb effort to hold the Soviets in check. Teller, a leading theorist on the hydrogen bomb, also pushed for a vigorous U.S. hydrogen bomb project. The surprise of the Soviet atomic test and the looming threat of a Soviet hydrogen bomb spurred the creation of a branch of Lawrence's Berkeley Radiation Laboratory in Livermore as a second U.S. weapons laboratory.

"If you know the enemy and know yourself, you need not fear the result of a hundred battles."

Sun Tzu, The Art of War
Circa 400 B.C.

As the 1950s progressed, *Sputnik*'s launch in 1957 and the perceived "missile gap" strengthened the drive for improved U.S. strategic forces and better understanding of Soviet capabilities. Over time, this need has expanded to include understanding the nuclear weapon capabilities, intentions, and motivations of other countries or groups hostile to the U.S. Intelligence analysis efforts at the Laboratory grew in response. With the end of the Cold War in 1992, Livermore Director John Nuckolls merged these efforts into the Nonproliferation, Arms Control, and International Security (NAI) Directorate. This new organization focused on the threat



posed by the proliferation of nuclear, chemical, and biological weapons—collectively called the weapons of mass destruction, or WMD.

Today, NAI researchers address the full spectrum of WMD proliferation issues—prevention, detection and reversal, response, and avoiding surprise.

Avoiding Surprise

After the Soviet Union's initial atomic bomb test, monitoring the Soviet weapons program became a paramount concern of U.S. intelligence agencies. In 1965, a formal relationship with the intelligence community was drawn up in a memorandum of understanding between the Central Intelligence Agency (CIA) and the Atomic Energy Commission (predecessor to the present-day Department of Energy). Livermore's Special Projects Group, known as Z Division, was established to provide the intelligence community with technical assessments of foreign nuclear programs and weapons capabilities. According to Dale Nielsen, the first Z Division leader, the division's initial charter was twofold. "We looked at the weapons fired by Russia, and later by China, to see what they were shooting, and we developed intelligence-related equipment as requested."

Z Division scientists gathered radiological samples from Soviet and Chinese nuclear tests, using technologies developed for collecting and analyzing atmospheric samples from U.S. tests. (See *S&TR*, June 2002, pp. 24–30.) They also developed new technologies for monitoring tests and collecting data that allowed analysts to tell what kind of weapons—atomic or thermonuclear—were being tested. Among the many intelligence-related systems, Nielsen recalls a clever "bug sniffer" designed by physicists and electronic engineers for detecting minute electronic monitoring devices. "The CIA wanted to test the system and told us, 'We've set up four bugs in a Virginia safe house. See if you can find them.' We gathered up the equipment, flew out there, and found five out of four. They never told us if that fifth was an actual part of the test."

As time went on, Z Division evolved to respond to the growing list of countries that concerned the nation's intelligence agencies. The division teamed regional and country-specific experts with weapons scientists and engineers to make analyses based on technical knowledge about nuclear weapons development and testing, specifics about each country's nuclear capabilities, and evaluation of nontechnical issues that motivate nuclear programs. Z Division also provided technical knowledge and intelligence information needed to control U.S. exports that could support WMD proliferation.

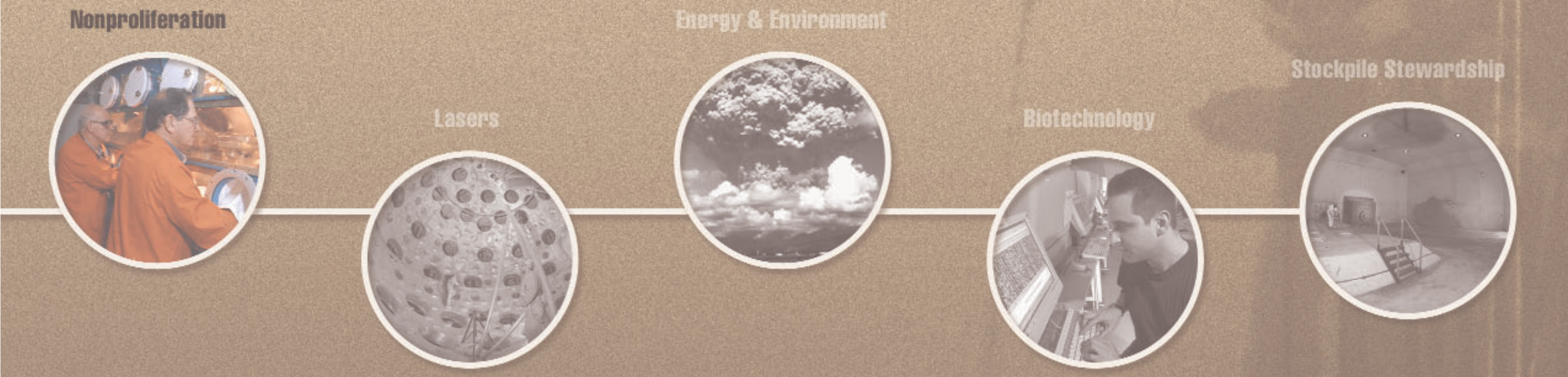
With the formation of the NAI Directorate, Z Division became the International Assessments Program and broadened its focus to include chemical and biological weapons proliferation. In addition, with the globalization of commerce and technology, Livermore's intelligence analysts recognized the need to assess the WMD capabilities of nonstate groups such as terrorists and patterns of cooperation among countries and groups of concern.

Researchers in the International Assessments Program are also addressing the national security implications of the U.S.'s rapidly growing reliance on critical networked infrastructures. The country—indeed the entire world—is becoming more dependent on computing, communication networks, and information technology. These researchers have developed a suite of sophisticated network analysis tools to assist government agencies in detecting, responding to, and preventing computer network attacks. Through this work, Livermore has become a national leader in information assurance technology.

Preventing Proliferation

The most effective way to prevent the spread of nuclear weapons is at the source, through treaties limiting or banning such weapons and, in the case of nuclear weapons, by securing weapons-usable nuclear materials. Material control is less effective in preventing the proliferation of chemical or biological weapons because the starting materials for these weapons have many legitimate uses.

The Laboratory first became involved in arms control in the 1950s. Public concern over atmospheric testing led the U.S. and the Soviet Union to establish a Conference of Experts to examine the technical issues associated with a comprehensive ban on nuclear weapons testing in all environments—the atmosphere, outer space, under water, and



under ground. Ernest O. Lawrence served as one of three U.S. representatives to this conference. Harold Brown, who became Livermore's director in 1960, was a member of the delegation's technical advisory group that developed a concept for verifying compliance with a comprehensive ban on nuclear weapons testing.

A number of Laboratory scientists participated in the technical working groups complementing the negotiations on a comprehensive test ban, examining ways to detect—and hide—explosions. Measuring seismic signals was seen as one technique for detecting underground explosions, and a worldwide network of seismic stations was built as part of this effort. (See box on p. 29.) However, Laboratory scientists were concerned that

The 1964 Salmon Event, a 5-kiloton detonation conducted 280 meters deep in a Mississippi salt dome, confirmed the theory of decoupling as a means of concealing clandestine nuclear explosions. In this photo, experimenters are lowering a canister containing the nuclear explosive for the Salmon Event.

a large cavity would reduce, or muffle, the shock wave by a factor of 30 to 50, essentially decoupling the strength of the seismic signal from the size of the explosion. The possibilities for such decoupling became a key issue in the U.S. negotiating position during early comprehensive test ban discussions. The Soviets' resumption of nuclear testing in September 1961 broke the bilateral moratorium and ended the negotiations at that time.

In the ensuing decades, Laboratory personnel continued to contribute to various arms control negotiations on both strategic force levels and nuclear testing. For instance, Livermore scientists participated in the technical working groups supporting Limited Test Ban Treaty negotiations and in the Nuclear Non-Proliferation Treaty. In the fall of 1977, negotiations on a comprehensive test ban resumed after a hiatus of many years. In the 1980s, issues regarding the verification of the Threshold Test Ban Treaty were resolved with the Joint Verification Experiment (JVE), a pair of nuclear tests jointly carried out at the U.S. and Soviet test sites. (See *S&TR*, June 1998, pp. 10–16.)

Geophysicist Eileen Vergino provided technical support to the U.S. delegates in Geneva during the treaty's protracted negotiations. Vergino remembers, "JVE was a turning point in Soviet relations with the West. Many American–Russian friendships were forged, and the more open atmosphere anticipated the post–Cold War era." In 1992, U.S. nuclear testing ceased, and the Comprehensive Test Ban Treaty was signed, although it has not been ratified by the U.S. Senate.

After the Soviet Union collapsed, the Lawrence Livermore, Los Alamos, and Sandia national laboratories established Lab-to-Lab interactions with the former Soviet nuclear institutes in former closed cities. The activities gave rise to a suite of cooperative programs with former Soviet laboratories to prevent the spread of weapons expertise or materials to other nations. (See *S&TR*, September 2000, pp. 4–11.) Through the Materials Protection, Control, and Accounting program, Livermore is working with several Russian sites to improve their protection of fissile materials and with the Russian Navy to strengthen the protection of fresh and spent fuel for its nuclear-powered vessels. The Laboratory is also working with the Russian Customs Service to curtail the smuggling of nuclear proliferation items by equipping high-risk border crossings with radiation detection equipment and training front-line customs officials in using the equipment.

In 2001, lengthy negotiations by Livermore scientists culminated in a formal agreement between a Russian weapons assembly facility and a medical equipment manufacturer to establish a commercial manufacturing facility at Sarov. This agreement was part of the Nuclear Cities Initiative, which seeks to create self-sustaining commercial enterprises for the closed cities, thereby helping to accelerate the downsizing of the Russian weapons complex and preventing displaced weapons workers from seeking employment with potential proliferators.

Detecting and Reversing Proliferation

To reverse proliferation of WMD requires detecting and identifying proliferation-related activities. If such activities are detected, the next step is to evaluate options for reversing the proliferation. Livermore provides expertise in this area by developing technologies to monitor and evaluate weapons proliferation activities and to protect critical U.S. facilities and troops from attack.

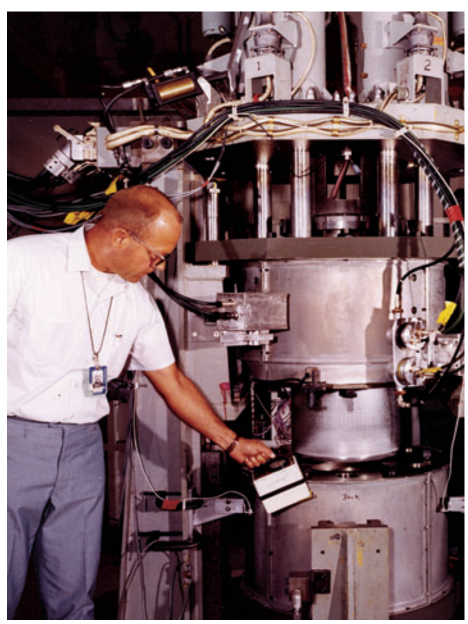
Predating this effort was work by Livermore weapons scientists who examined the consequences of various "us-versus-them" scenarios. By the mid-1960s, with the large buildup of Soviet nuclear weapons and delivery systems, the U.S. faced some serious "what-if" questions. If a nuclear exchange occurred between the U.S. and the Soviet Union, U.S. warheads would have to contend with defensive countermeasures such as a nuclear-tipped interceptor or antiballistic missile, which could deliver a blast aimed at destroying or disabling a U.S. warhead before it reentered the atmosphere. Would such a countermeasure work? Nobody knew for certain. The Super Kukla reactor at the Nevada Test Site was designed to find out. Super Kukla, an ultrahigh prompt burst reactor, produced an intense pulse of neutrons and gamma radiation to simulate the environment a U.S. ballistic missile warhead might encounter during enemy countermeasures—in essence, a nuclear blast without the blast.

This focus on nuclear effects was one mission of D Division, which was also tasked with anticipating the strategic and tactical needs of the U.S. military services. In an effort to meet these needs, the Laboratory developed an early presence in the arena of computer-driven conflict simulation. Since the mid-1970s, Livermore computer scientists have led in the development of increasingly realistic software to simulate the tactical battlefield. "At first, you had to program the orders of the opposing force into the computer ahead of time, which didn't make for a very realistic scenario," recalls Paul Chrzanowski, who joined D Division in 1977 and became its leader in 1982. "Then George Smith, a very creative guy, developed a simulation in which two opposing players observe the battle on separate computer monitors and give orders."

The Laboratory's landmark Janus program, developed in the late 1970s, was the first conflict simulation tool that was real-time player-interactive and used a graphical user interface. Livermore simulations were employed in Operation Desert Storm in the Middle East as well as in combat planning for Somalia, Bosnia, and other international trouble spots. In 1997, a team of NAI computer scientists unveiled Joint Conflict and Tactical Simulation (JCATS), the culmination of more than two decades of computer-driven mission analysis and rehearsal experience. (See *S&TR*, November 1996, pp. 4–11; June 1999, pp. 4–11; January/February 2000, pp. 4–11.)

A more recent computer-driven innovation developed for the U.S. military is the Counterproliferation Analysis and Planning System (CAPS), which is widely used by military planners to evaluate the WMD production capabilities of a country of concern and assess interdiction options. Drawing on information

Livermore provided key support in upgrades made on four nuclear refueling ships for the Russian icebreaker fleet and the Russian Navy. The upgrades improve the protection of fresh, highly enriched reactor fuel for the nuclear-powered vessels. Work such as this involves direct interactions with the Russian Ministry of Defense, an activity that would have been inconceivable during the Cold War.



The Super Kukla reactor, operated at the Nevada Test Site between 1965 and 1978, simulated the hostile environment of a nuclear exchange. Nuclear weapon components and materials were placed inside an experiment cavity, and instruments measured how well the tested samples stood up to the hostile radiation environment.

from multiple sources, CAPS can model the various processes—chemical, biological, and metallurgical—that are used to build WMD and delivery systems. CAPS identifies critical processing steps or production facilities which, if denied, would prevent that country from acquiring such weapons.

Responding to Threats

When—despite everything—bad things happen, the Laboratory has the personnel and the science and technology to help the nation respond.

(a)

(b)

(a) In the mid-1970s, the Janus code developed at the Conflict Simulation Laboratory ran an early, very simple conflict simulation. (b) Today, the Livermore-developed Joint Conflict and Technical Simulation (JCATS) models are used by the U.S. military commands and services and various U.S. security forces for training, tactical analysis, and mission planning for battlefield and urban conflict situations.

Since the early 1970s, Livermore has coordinated its responses to off-site nuclear emergencies through NEST—the Nuclear Emergency Search Team. When the Soviet satellite Cosmos 954 fell to Earth in northern Canada in 1978, Laboratory researchers tracked the reentry path, provided estimates of reentry location, and participated in a multinational effort to locate and retrieve radioactive debris. Members of NEST—health physicists, chemists, nuclear physicists, and engineers—hauled radiation detectors, liquid nitrogen, sample containers, power generators, portable computers, and even a helicopter to a desolate area populated only by caribou and Inuit hunters. The international team successfully found hundreds of very small pieces Cosmos left that survived reentry, and Livermore researchers identified the reactor fuel and estimated the fission-product inventory.

In addition to NEST, Laboratory employees also participate in the Radiological Assistance Program, which helps deal with civilian incidents involving radioactive materials; in the Accident Response Group, which responds to accidents involving a U.S. nuclear weapon; and in the Joint Technical Operations Team, a nuclear response team that assists the Department of Defense in dealing with terrorist nuclear devices.

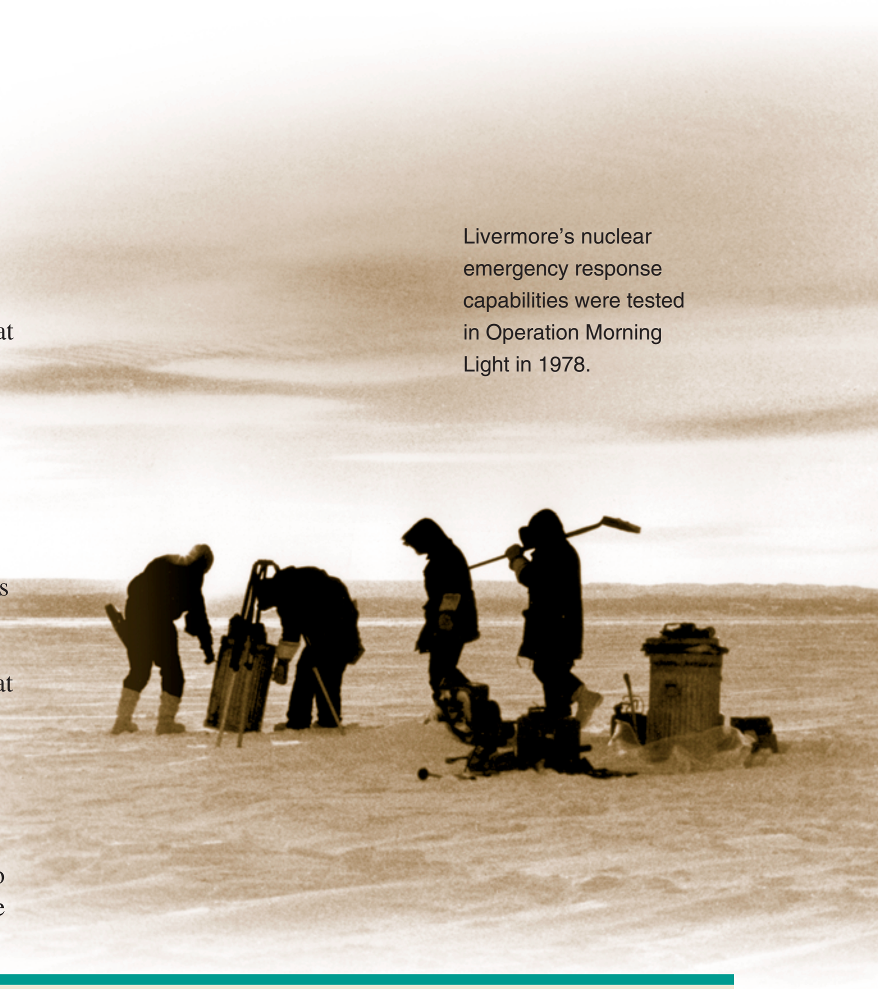
Livermore's NAI directorate is home to a number of technologies and capabilities that address the response end of the threat spectrum. In the Forensic Science Center, for example, experts in organic and inorganic chemistry and biochemistry determine the composition and often the source of minute samples of materials. (See *S&TR*, April 2002, pp. 11–18.) A major effort since the center's founding in 1991 is the development or adaptation of forensic analysis technologies for field use. In 1994, the Department of Energy asked the center to help investigate two gaseous-diffusion uranium enrichment plants that would be subject to international inspections. (See *S&TR*, August 1995, pp. 24–26.) DOE wanted to know whether an inspector could walk through a plant, surreptitiously collect samples of material, and later replicate the enrichment process. In 1998, the center used its portable thin-layer chromatography system, which can simultaneously analyze 100 samples, in the field for the first time to examine more than a thousand World War II munitions that had been unexpectedly unearthed. (See *S&TR*, December 1998, pp. 21–23.)

For almost a decade now, Laboratory researchers, working on the "when" rather than "if" premise, have been developing systems to rapidly detect and identify biological warfare agents including anthrax and plague. In 1999, Livermore scientists and engineers unveiled the Handheld Advanced Nucleic Acid Analyzer (HANAA), the first truly portable battery-powered device for identifying bioagents in the field. HANAA can analyze samples in less than 30 minutes, compared to the hours or days that regular laboratory tests typically require. (See *S&TR*, January/February 2002, pp. 24–26.) Another device, the Autonomous Pathogen Detection System (APDS), is being designed to continuously monitor the air for pathogens as a sort of biological smoke alarm for airports, stadiums, or conference halls.

Ron Koopman, an associate program leader with the Chemical and Biological National Security Program, notes that the availability of HANAA and APDS owe much to forward-thinking efforts begun in the previous decade. "A number of people recognized the vulnerability of the country to bioterrorism a long time ago," he says. "Back then, although bioterrorism seemed far away and was something we hoped would never happen, the Laboratory and members of the defense community decided to invest in the research. Thanks to that investment, we now have something to put in the hands of people to protect us all, something that can help during the current crisis and in the long run."

Laboratory scientists also worked with their counterparts at Los Alamos to develop the Biological Aerosol Sentry and Information System. This system, which reduces the time for detecting a bioagent release from days or weeks to less than a day, was deployed as part of the security strategy for the 2002 Winter Olympics in Salt Lake City.

Biodetectors require unique DNA sequences or antibodies to identify and characterize pathogens. Researchers at Livermore



Livermore's nuclear emergency response capabilities were tested in Operation Morning Light in 1978.

Detecting Clandestine Nuclear Tests and Verifying Treaties: Two Sides of the Same Coin

Lawrence Livermore scientists have long played an important role in providing monitoring technology that supports test ban treaty verification and site inspection. On September 19, 1957, the Laboratory detonated the first contained underground nuclear explosion, Rainier, in a tunnel at the Nevada Test Site. The Rainier Event was announced in advance so that seismic stations throughout the U.S. and Canada could attempt to record a signal. Information from this event ultimately led to an array of seismic detectors for monitoring nuclear test activities worldwide, as part of the Limited Test Ban Treaty.

Nearly 35 years later, when the world received news of the Indian and Pakistani clandestine underground nuclear tests, Livermore researchers used the tests to validate modern seismic methods they had developed to monitor the Comprehensive Test Ban Treaty. (See *S&TR*, September 1998, pp. 4–11.) Using data recorded worldwide by a host of seismic monitoring stations, the team successfully differentiated the nuclear blasts from typical regional earthquakes, characterized the yields of the tests, and noted inconsistencies between the announced test yields and the seismic data. The seismic signals from the nuclear tests provided important new data for calibrating seismic stations in important regions of the world.

Livermore researchers have also developed on-site inspection procedures and technologies for collecting samples of soil, gases, and water to look for radioactive materials and for identifying underground explosion cavities or rubble. In the early 1990s, a team led by geophysicist Charles Carrigan theorized that highly sensitive instruments might be able to detect small amounts of rare, radioactive gases generated in underground nuclear detonations. In 1993, a chemical explosion called the Non-Proliferation Experiment was conducted at the Nevada Test Site to simulate a 1-kiloton underground nuclear detonation. Results from the experiment and computer simulations imply that sampling soil gases for rare, explosion-produced radioactive tracer gases at the surface near a suspected underground test could help detect nearby underground nuclear explosions that do not fracture the surface, even several months after the test. (See *S&TR*, January/February 1997, and elsewhere are developing a comprehensive array of such signatures. One effort focuses on analyzing the genome of the various strains of the bacterium that causes plague. Laboratory researchers are searching for the DNA sequences that are unique to all strains of the pathogen but are not found in any of its close relatives. (See *S&TR*, March 2002, pp. 4–9.)


In a project for the U.S. Army in 1998, Livermore's Jeff Haas examined more than 1,200 mortars in two days using the Forensic Science Center's thin-layer chromatography screening system.

Facing the Threat, Knowing the Enemy

"Over the years, researchers at the Laboratory have had the foresight to analyze and prepare for many versions of the 'catastrophic maybe,'" says NAI Associate Director Wayne Shotts. For most of the Laboratory's existence, the consuming national security threat to the U.S. was the nuclear arsenal of the Soviet Union. The energies, talent, and resources of the national security laboratories were dedicated to checkmating the Soviet threat. "That world," notes Shotts, "no longer exists." Today, the most serious threat arises from the proliferation of nuclear, chemical, and biological weapons, and the very real threat of terrorism using those weapons. In a development that defines the national focus on this growing threat, NAI has broken ground for a new building—the International Security Research Facility. According to Bruce Tarter, who recently stepped down as Lawrence Livermore's director, this building will serve as the Laboratory's "command post for connectivity to Washington" and its efforts to fight WMD proliferation and terrorism.

Through NAI, the Laboratory applies its nuclear weapons expertise, developed through its historical weapons program and continuing stockpile responsibilities, to the challenge of nuclear nonproliferation. In addition, NAI draws on the Laboratory's chemical and biological expertise to help stop the spread of chemical and biological weapons. From one end of the threat spectrum to the other—prevention, detection and reversal, response, and avoiding surprise—Livermore stands ready to help the nation face the threat and know the adversary.

—Ann Parker

Key Words: biodetection, biological and chemical weapons, conflict simulation, Comprehensive Test Ban Treaty, forensic analysis, nonproliferation, seismic monitoring, treaty verification, weapons of mass destruction (WMD).

For more information about the Nonproliferation, Arms Control, and International Security Directorate, see:

www.llnl.gov/nai/nai.shtml

For further information about the Laboratory's 50th anniversary celebrations, see:

www.llnl.gov/50th_anniv/

This Model Can

A new computer program simulates the physics of fire and weather patterns to help combat wildfires.

THE destructive wildfires in Colorado, Oregon, Arizona, and California this summer were searing reminders that uncontrolled fires in forests and brushlands pose an increasing threat to life, property, and natural resources. After 100 years of fire suppression activities, combined with unusually hot and dry weather patterns, dangerous amounts of highly flammable fuels have accumulated throughout the nation.

As a result, millions of acres of forests and brushlands and thousands of homes are at high risk. The problem is exacerbated as people continue to relocate from urban to rural areas and homes and communities are built adjacent to state and national forests.

"The nation's capability to respond to wildfires is becoming overextended," says Livermore atmospheric scientist Michael Bradley. "It is essential that we do all we can to ensure firefighters' safety and increase their ability to efficiently limit the spread of potentially devastating fires."

Bradley notes that fire managers have an arsenal of weapons at their disposal, ranging from aerial tankers to small armies of dedicated firefighters. One weapon that is lacking, however, is a physics-based computer simulation system that can accurately predict wildfire behavior for specific weather conditions, types of vegetation, and terrain. Such a capability would help fire managers to plan for different fire scenarios, anticipate where and how quickly a fire will spread, and evaluate the effectiveness of alternative firefighting strategies. With this modeling capability, fire managers could use their limited personnel and equipment much more effectively, thereby saving lives, property, and irreplaceable natural resources.

Such a simulation capability is being developed for the first time by a team of researchers from Lawrence Livermore and Los Alamos national laboratories. Supported by Laboratory Directed Research and Development funds, the project combines a physics-based

Take the Heat

wildfire model developed at Los Alamos with the extensive emergency response capabilities of the National Atmospheric Release Advisory Center (NARAC) at Livermore, including its weather prediction and smoke transport codes and Livermore's supercomputers. The effort combines the special capabilities and resources of the two laboratories, says Bradley, who leads the Livermore effort that also includes atmospheric scientists Charles Molenkamp and Martin Leach and geographical information systems (GIS) experts Charles Hall, Lee Neher, and Lynn Wilder.

Predicting wildfire behavior is not a new concept. The models most widely used by firefighters, however, are relatively unsophisticated programs based on data obtained by laboratory experiments, for example, the burn rate of pine needles in wind tunnels. Such experimental results for a variety of vegetative fuels are used in look-up tables to estimate burn rates based on the total amount of fuel, wind speed, and the slope of simplified two-dimensional terrain. The model is then used to predict wildfire behavior, guide firefighting tactics, and assist in training and planning.

"Current models do not account for the many complex physical processes that characterize real wildfires and determine their behavior," says Bradley. The models also don't reflect how the terrain and vegetation change (sometimes dramatically within a few meters), how the weather changes, and, perhaps most importantly, how the fire and weather continuously interact.

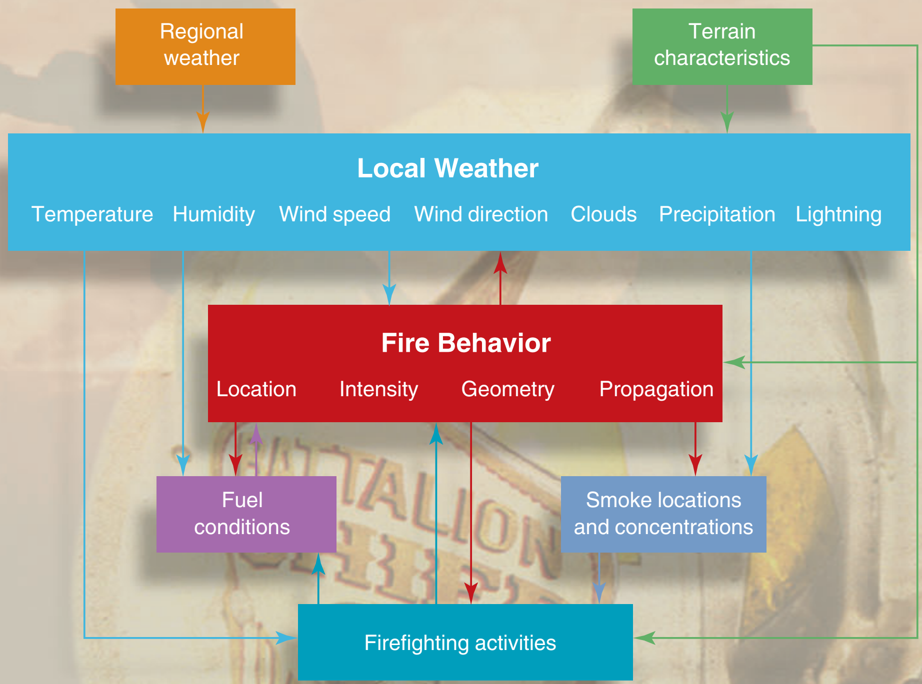
Winds, air temperature, humidity, and precipitation, for example, influence the flammability of fuel and largely determine the risk of fire ignition. In addition, wind speed and direction determine the rate of fire spread and the amount of transported embers from which new fires can be ignited. Weather conditions also determine the location and concentration of smoke plumes, which can interfere with ground and aerial firefighting operations and cause health hazards downwind.

In turn, the heat from wildfires causes rising air currents that strongly modify local weather patterns and create rapidly changing winds that may fan the fire. As a fire approaches, unburned vegetation preheats and dries and ignites more easily. All of these interacting physical processes are reflected by the Livermore–Los Alamos computer model.

Model Starts with FIRETEC

The basic fire-simulation code, called FIRETEC, has been developed over the past 7 years by a Los Alamos group headed by atmospheric scientist Rod Linn. The group experienced first-hand the destructive power of wildfires in 2000, when the Cerro Grande fire ripped through the Santa Fe national forest as well as parts of the town of Los Alamos and the Laboratory itself.

FIRETEC simulates the mechanisms of fire propagation in ways that far exceed the capabilities of wildfire models currently in use. FIRETEC predicts the spread of wildfires based on a fundamental treatment of physical processes such as combustion and turbulence and uses a terrain-following coordinate system based on digitized maps. It takes into account the two basic heating mechanisms of fire: the turbulent convective motion of heated air and the infrared radiation emitted by the fire. Using spatial resolutions of 1 to 10 meters, FIRETEC also tracks the



Existing wildfire models, using data from isolated laboratory experiments, do not adequately represent the complicated, interactive processes of wildfires defined in this diagram.

depletion of fuels and oxygen during combustion.

The code realistically represents the vegetation of an area, including the mixture of species, their densities, and their three-dimensional structure. Because the code includes a vertical fuel representation, it differentiates between grass, tree trunks, and tree crowns, thereby making simulations much more realistic. This degree of realism is needed because in some situations grass will burn without the fire spreading to tree crowns, whereas in other situations, the crowns ignite. In simple models, says Bradley, fuel is simply "flat," represented by a calculated number of tons of vegetation per acre, with no vertical structure.

To account for the interactions between fire and atmosphere, the Los Alamos group combined FIRETEC with the fine-resolution, high-gradient flow solver program known as HIGRAD, which was developed by Jon Reisner. HIGRAD delivers accurate atmospheric simulations at extremely high spatial (1 meter) and temporal (thousandths of a second) resolution.

HIGRAD, however, cannot represent the regional weather patterns within which wildfires burn. "HIGRAD simulates close-in air flow over small regions of a fire but does not take into account more remote weather processes such as cold fronts, high- and low-pressure systems, and precipitation that develop over much larger geographical areas," says Bradley.

Adding Regional Weather

To overcome this limitation, the team incorporated the Coupled Ocean–Atmosphere Mesoscale Prediction System (COAMPS), developed by the U.S. Naval Research Laboratory in Monterey, California, and later refined by NARAC scientists. COAMPS is run twice daily by NARAC to predict regional weather at scales ranging from about 1,000 kilometers down to a few kilometers. The Livermore wildfire team has run COAMPS using horizontal resolutions as fine as approximately 150 meters. COAMPS predicts winds, temperature, pressure, humidity, and precipitation for several days. The code is formulated in terrain-following coordinates, which are advantageous for atmospheric simulations over rugged terrain. "COAMPS provides the regional atmospheric environment within which HIGRAD–FIRETEC simulations run," explains Bradley.

He says that integrating HIGRAD–FIRETEC with NARAC's capabilities provides access to a wide range of resources that strengthen the wildfire simulation capability. These resources include a detailed global terrain database, global mapping system, global weather data acquisition system, and weather prediction systems. NARAC is supported by vast quantities of meteorological data that are collected daily—and sometimes hourly—from around the world.

NARAC also has the leading atmospheric smoke dispersion simulation model, called ARAC-3. Although the model was originally conceived to track radionuclide releases, the center can use it to respond to atmospheric releases of other materials, including toxic chemicals, biological agents, ash from volcanic eruptions, and, most relevantly for firefighting, smoke. Following Operation Desert Storm, NARAC provided twice-daily predictions of smoke dispersion from the burning oil wells in Kuwait. More recently, it predicted the dispersion of smoke from two massive tire-dump fires near Tracy and Wesley, California, from which smoke rose to almost 2,000 meters above ground level. (See *S&TR*, June 1999, pp. 4–11.)

Livermore also offers substantial supercomputer resources. Computer models that accurately predict the behavior of wildfires require enormous processing power that currently can only be provided by massively parallel

The Claremont Resort narrowly escaped destruction during the 1991 wildfire in the hills of Oakland and Berkeley, California.

supercomputers (machines using many processors in tandem). Wildfire simulations performed at Livermore, for example, typically use 64, 64-bit processors belonging to Livermore's TeraCluster2000 680-billion-operations-per-second (gigaops) supercomputer.

Modeling Threats and Responses

Throughout the simulation program's development, the Livermore–Los Alamos team has conferred with federal, state, and local fire managers. Many valuable suggestions have been incorporated into the program's capabilities, and several applications have emerged.

Two applications—wildfire preparedness planning and long-term planning for communities and wildland management—are available now. With adequate funding, three additional applications—analyzing specific fire threats, predicting fire behavior for prescribed burns, and training firefighters—could be ready next summer. The ultimate goal, real-time firefighting support, is several years away and awaits the development of even more powerful computers for faster turnaround.

The wildfire preparedness planning application permits realistic simulations of past or hypothetical future fires for specific locations, with high-resolution modeling of terrain, types of vegetation, and weather conditions. "This is a powerful tool for community fire preparedness planning," says Bradley.

The long-term planning application permits evaluation of vegetation management options such as thinning trees or designing fuel breaks. Such planning is especially important at the urban–wildland interface in determining the fire threat to new homes, commercial development, and open areas.

Fire behavior predictions for prescribed burns would be available to fire managers a few hours before they ignite the fuel. This advance knowledge would enable managers to decrease the risk of prescribed burns going out of control (such as happened with New Mexico's Cerro Grande wildfire) and of violating air quality standards.

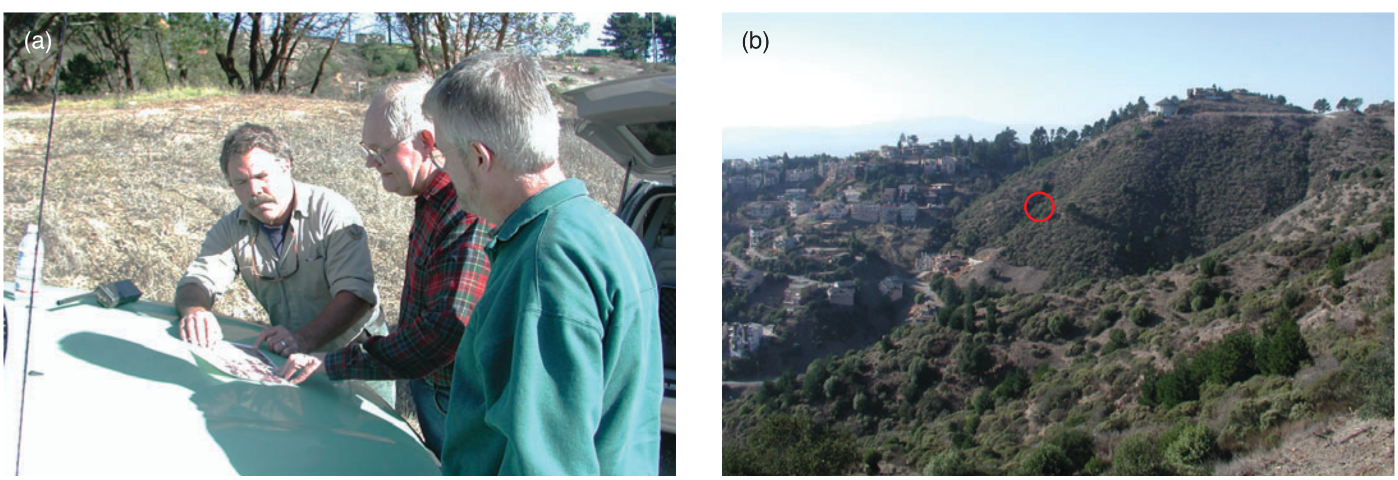
Fire threat analyses would produce physics-based predictions of potential fire behavior for specific locations with a few days' notice. This feature would be particularly useful to fire managers in assessing the relative risks of fire breaking out at various locations during periods of increased threat.

As a training tool, the program would be unsurpassed at showing how different factors affect the behavior of wildfires. After specifying the exact ignition point of a fire, students could vary the weather, vegetation, fuel conditions, and firefighting methods to understand their effects. "We envision this application serving a role similar to that of a flight simulation program," says Bradley. "Students could make mistakes without risking their lives."

The program's ultimate goal is real-time support for firefighters. In this application, the program would help fire managers to make critical operating decisions regarding the deployment of firefighters and equipment. The program could also predict the relative effectiveness of various firefighting procedures, such as fuel breaks, backfires, air tanker fire-retardant drops, and helicopter water drops.

Model Validation Essential

The team has been validating the program by simulating well-documented wildfires. An early



(a) East Bay Regional Parks ranger Bill Nichols (left) and Livermore researchers Charles Molenkamp (center) and Michael Bradley used global positioning system tools to determine for the first time the ignition points of the 1991 fire in the Oakland–Berkeley hills. (b) The ignition point for the second fire (which began Sunday, October 20, 1991) in Tunnel Canyon is circled.

simulation using HIGRAD–FIRETEC successfully re-created the Corral Canyon wildfire that occurred in Calabasas, near Malibu, California, on October 22, 1996. The fire had been smoldering in the riparian (vegetation along a gully) area at the bottom of a canyon. It suddenly rushed up one side of the canyon, catching firefighters off guard and injuring several. The simulation re-creates the rapid spread of the fire, from the bottom of the drainage area to the crest of the hill, within 28 minutes, about the time the actual fire took. By comparison, a simulation of the same fire with a traditional model predicts that it would take about 6 hours to burn the same area. The difference between the two simulations is the interplay among the terrain, fire, and winds that is represented by HIGRAD–FIRETEC.

"Firefighters sometimes think they have a lot of time when they really don't," says Bradley. The Corral Canyon simulation showed that strong sea breezes channeled by the terrain pushed the fire up the hill much faster than the firefighters thought possible.

The model also shows that if the riparian vegetation were replaced with dry grass, the fire spreads up both sides of the canyon. "The simulation results are encouraging because they compare so well with field observations," Bradley says.

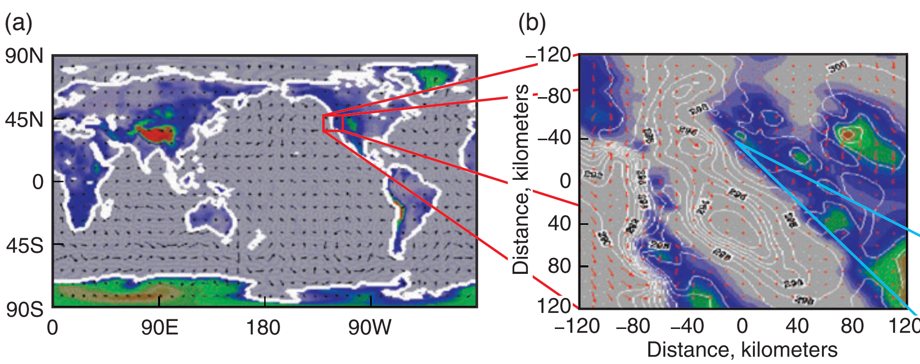
To provide a more exhaustive validation of the program's capabilities, Bradley and his group, together with Livermore GIS experts, have been reconstructing the early stages of the catastrophic 1991 fire in the hills of Oakland and Berkeley, California, and are looking at current fire dangers to neighborhoods that escaped the conflagration. Bradley is sharing the results with East Bay fire agencies, the city governments of Oakland, Berkeley, and El Cerrito, the East Bay Regional Park District, the East Bay Municipal Utilities District, the University of California at Berkeley, Lawrence Berkeley National Laboratory, and the California Department of Forestry and Fire Protection.

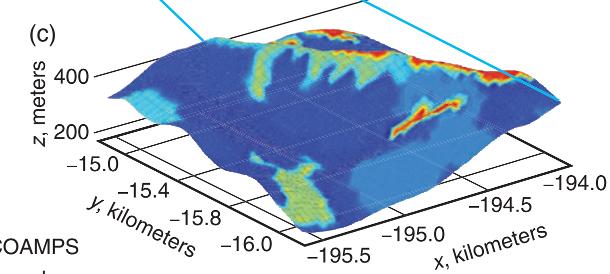
The Oakland–Berkeley hills fire claimed 25 lives and destroyed more than 3,000 dwellings. The simulations re-create its start at about 11 a.m. on Sunday, October 20, 1991, in Tunnel Canyon. (One day earlier, a small grass fire occurred about 100 meters from the ignition point of Sunday's fire. Embers from Saturday's fire, at first thought to have been extinguished, almost certainly started the Sunday conflagration.)

Working with the East Bay Regional Park District, the Livermore group produced the first global positioning satellite coordinates for the ignition points of the Saturday and Sunday fires. Next, the team built a virtual atmosphere for October 20, 1991, by using historical weather data provided by the European Center for Medium Range Weather Forecasting. The data, which had a resolution of about 120 kilometers, were fed into COAMPS to simulate the humidity, temperature, wind direction, and wind speed over the area of the incipient wildfire.

Re-creating Front Yard Weather

The COAMPS data were used by HIGRAD to simulate fine-scale weather at 10-meter resolution. "At this resolution, we're actually simulating the weather that occurred in the front and back yards of individual homes in the Oakland–Berkeley hills," notes Bradley. Volumes of detail on the terrain and vegetation were fed into FIRETEC





The wildfire modeling capability zooms down to extremely fine resolution. For the Oakland–Berkeley hills fire that began October 20, 1991, the team constructed (a) a virtual atmosphere by using historical weather data provided by the European Center for Medium Range Weather Forecasting. The data, which had a resolution of about 120 kilometers, were fed into the Coupled Ocean–Atmosphere Mesoscale Prediction System (COAMPS) to simulate (b) the humidity, temperature, wind direction, and wind speed over the San Francisco Bay Area. The COAMPS data were used by the high-gradient flow solver (HIGRD) program to simulate (c) fine-scale weather at 10-meter resolution over the Oakland–Berkeley hills.

along with the dimensions of a football-shaped scar on the hillside, which resulted from the Saturday fire.

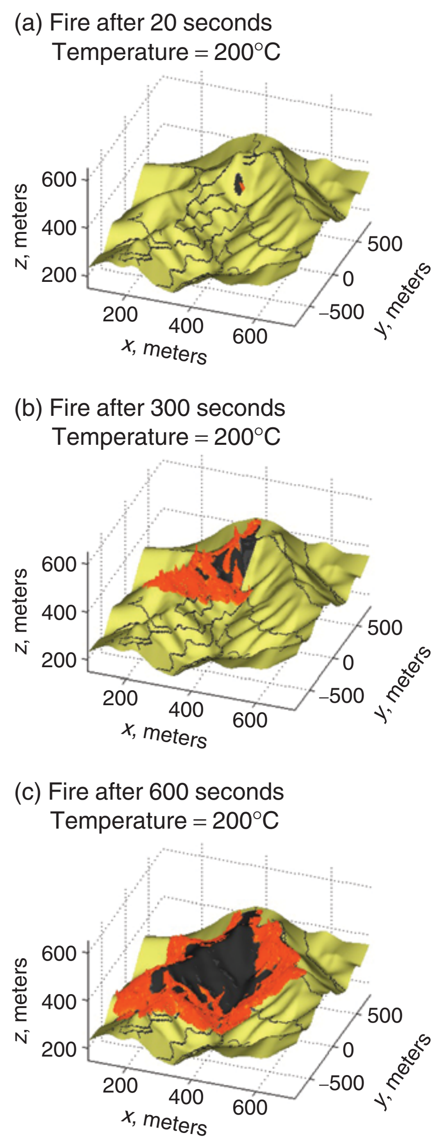
The fire was "lit" in the FIRETEC program by raising the temperature by 100°C at the exact ignition location determined earlier by the Livermore team. The simulation shows wind-whipped flames quickly spreading outward from the ignition point throughout Tunnel Canyon, which contained bone-dry trees, bushes, and grasses. Other aspects of the simulation show the direction and speed of winds (as affected by the fire) and the percentage of vegetation burned.

Bradley says that a common reaction to watching the simulations is that the fire spreads unrealistically fast, but fire officials who have seen the simulation say it is an accurate representation of what happened. "Conditions were nearly perfect for a devastating fire," Bradley says.

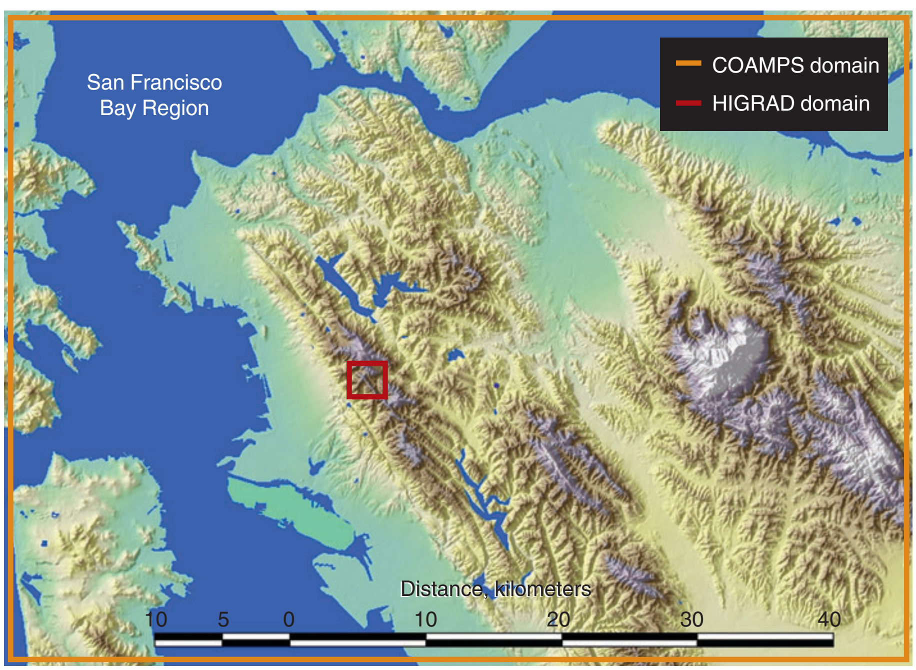
As with the Calabasas fire simulation, the Oakland hills model shows that the exact ignition location is important. If Sunday's ignition point is moved only 100 meters away, to the other side of the canyon, the fire follows a different course.

The team has also developed a fire consequence analysis capability by meshing model results with data maps created with computerized GIS tools. (See *S&TR*, September 2002, pp. 10–16.) GIS analyses make the program more useful to fire chiefs and other emergency planners by superimposing layers of digitized visual information over the simulation. The GIS map layers include roads, schools, fire stations, electrical transmission lines, and even the location of fire hydrants. A GIS layer of land parcel maps, for example, allows users to select specific homes and determine their vulnerability to wildfires.

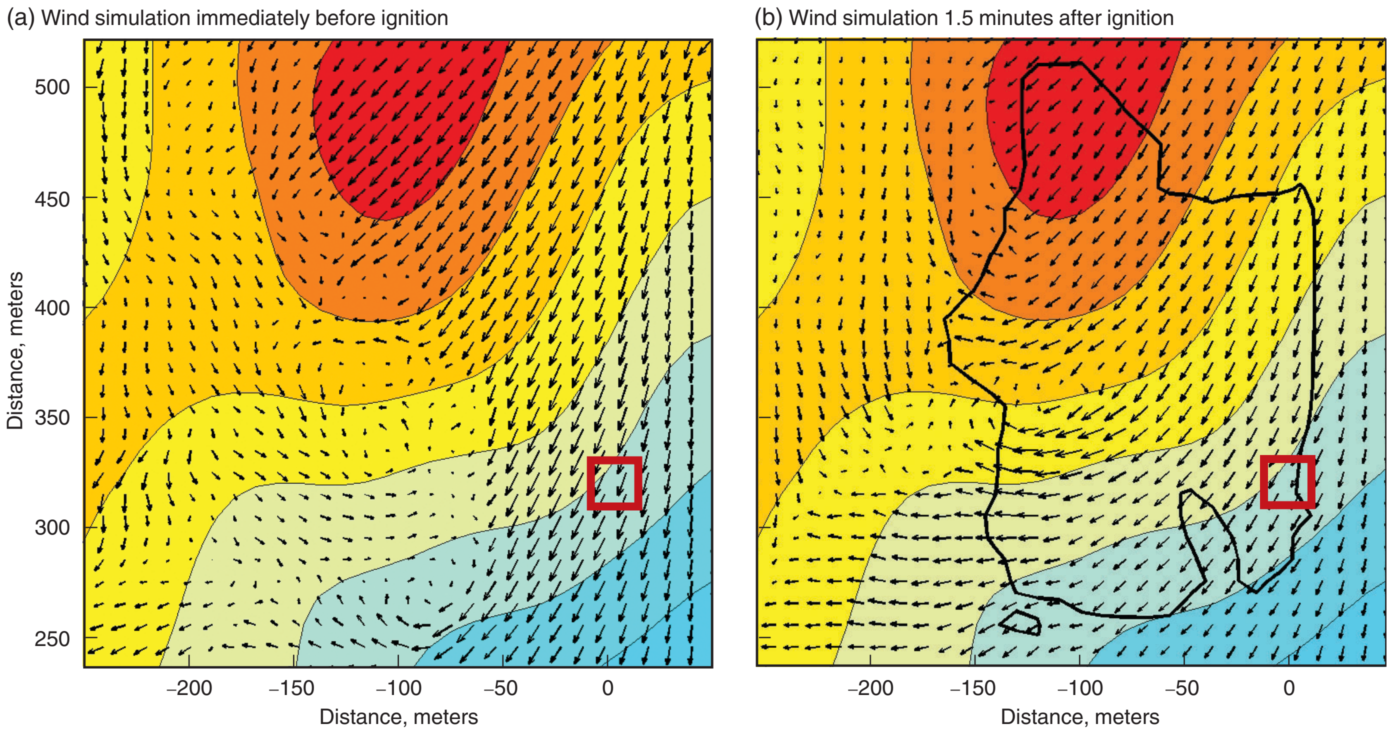
By combining the wildfire models with GIS tools, says Bradley, fire chiefs and analysts can plan the best routes for



A sequence of three frames taken from the computer simulation of the Oakland–Berkeley hills fire, which started in Tunnel Canyon. (a) A football-shaped dark area corresponding to Saturday's extinguished fire can be seen. Sunday's fire broke out just 30 meters away. (b) Three-hundred seconds (5 minutes) later, the fire is spreading quickly up the canyon. (c) Six-hundred seconds (10 minutes) after ignition, the fire has spread



A topographical map of part of the greater San Francisco Bay Area. The Coupled Ocean–Atmosphere Mesoscale Prediction System (COAMPS) weather prediction code modeled the larger area, while the high-gradient flow solver code (HIGRAD) is restricted to a 1.6-square-kilometer area directly over the Oakland–Berkeley hills fire.



(a) A simulation of the wind with 10-meter resolution immediately before ignition of the Oakland–Berkeley hills fire. The arrows' directions indicate wind direction, while the arrows' lengths indicate wind speed. The red box is the fire's ignition site. (b) One and one-half minutes after ignition, winds are significantly altered by the fast-moving fire (perimeter is outlined).

firefighters to take as well as the safest evacuation routes for residents at risk. Planners can also readily determine the effects of thinning stands of trees or building fire breaks.

The Livermore group is particularly interested in areas in the Oakland and Berkeley hills that didn't burn in 1991 and that contain a substantial amount of vegetation, homes, and research facilities. The group hopes to evaluate the effectiveness of fuel breaks and other vegetation management techniques for areas that escaped the 1991 fire. It also hopes to simulate wildfires in Claremont Canyon and in Strawberry Canyon, the site of Lawrence Berkeley National Laboratory, the Lawrence Hall of Science, and a portion of the University of California at Berkeley campus. These simulations will not only help the group to further understand and improve the model, but they will also provide valuable information for local agencies.

Bradley notes that the Oakland and Berkeley hills areas are telling examples of the dangers posed by the urban–wildland interface, where homes are nestled within thick vegetation.

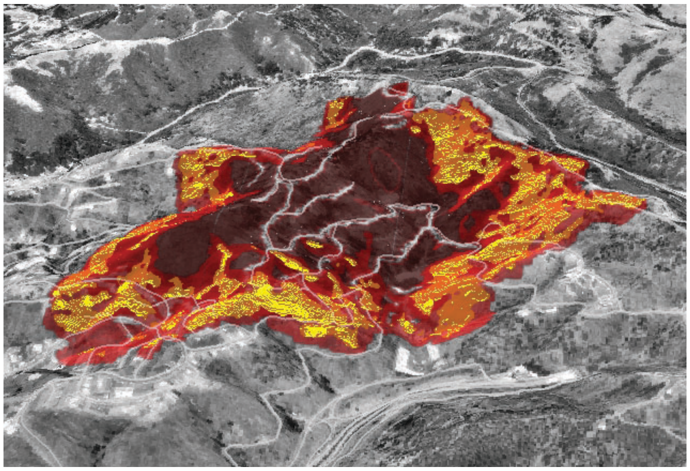
Chance to Make History

Because prescribed burns are planned far in advance, they provide the best opportunity for validating the program's accuracy. The burn location and ignition time are known before the burn occurs; the amount, type, and moisture content of vegetation are calculated before ignition; the weather conditions are known; and the behavior of the fire can be documented.

Bradley has successfully simulated smoke dispersion from several prescribed burns that were conducted at Site 300, Livermore's remote research facility. The simulations used the ARAC-3 dispersion model and compared well with observations of the smoke plume. He is hoping to use the full predictive power of the Livermore–Los Alamos model to provide reliable estimates of the fire behavior and smoke dispersion at least 24 hours before the prescribed burns are ignited at Site 300 in 2003.

"By next summer, it is possible we will be able to run the system fast enough to predict the first 30 minutes or so of the fire's behavior during a prescribed burn. If we are successful,

(a)



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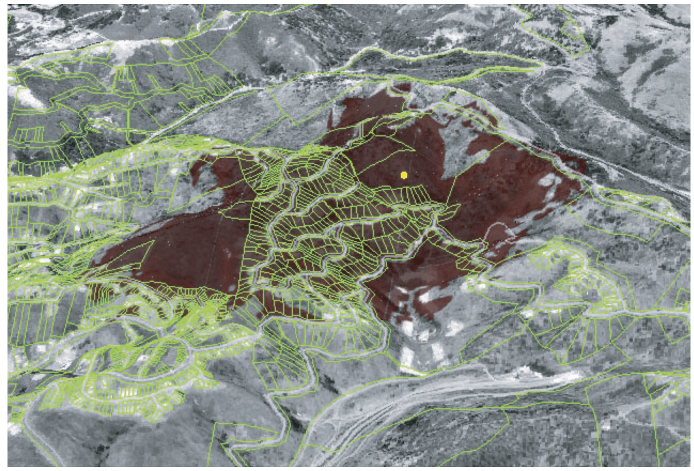


These images combine the result of (a) a computer simulation of an early stage of the Oakland–Berkeley hills fire with (b) a geographical information systems map of land parcels in the Oakland–Berkeley hills. Any home on the land parcel map can be selected to determine its address and its risk from a fire.

it will be a truly historic event for fire science.” The team also has received several offers from fire management agencies to participate in their prescribed burn programs.

Enthusiastic Reception

The concept of an advanced wildfire simulation capability has been received positively by potential users. As the program’s development has progressed, an increasing number of agencies have expressed interest in the project, including the Los Angeles County Fire Department, the nation’s largest. In October, the University of California sponsored a wildfire physics workshop that explored how other scientists and fire managers can use the Livermore–Los Alamos program as the basis for advanced wildfire behavior studies. “We want to build a community of scientists and firefighters,” says Bradley. A second workshop is planned for early next year.

The team is looking at the current program as a central core to which additional modules can be added to strengthen its overall capabilities. For example, the increasing threat of wildfire at the wildland–urban interface makes it appropriate to include structures such as homes and businesses in the simulation system. The team is in contact with researchers at the National Institute of Standards and Technology who are developing a code that simulates burning structures. Developing such a code is a substantial task because of variations in structural materials and their contents.

A module to represent the process of fire spreading by showers of embers, called spotting, will be added to HIGRAD–FIRETEC next year. The team is collaborating on the module with researchers at the University of California at Berkeley. “This is not as simple as it might sound,” Bradley comments. “We have to decide on the embers’ sizes, how far the winds take them, and the percentage of times they start new fires.”

Eventually, the team foresees a 24-hour national wildfire prediction program being established, with fire managers and even firefighters in the field linked to NARAC with laptop computers.

Putting wildfire simulation on a solid physics-based footing can only be good for firefighters, the public, and the environment.

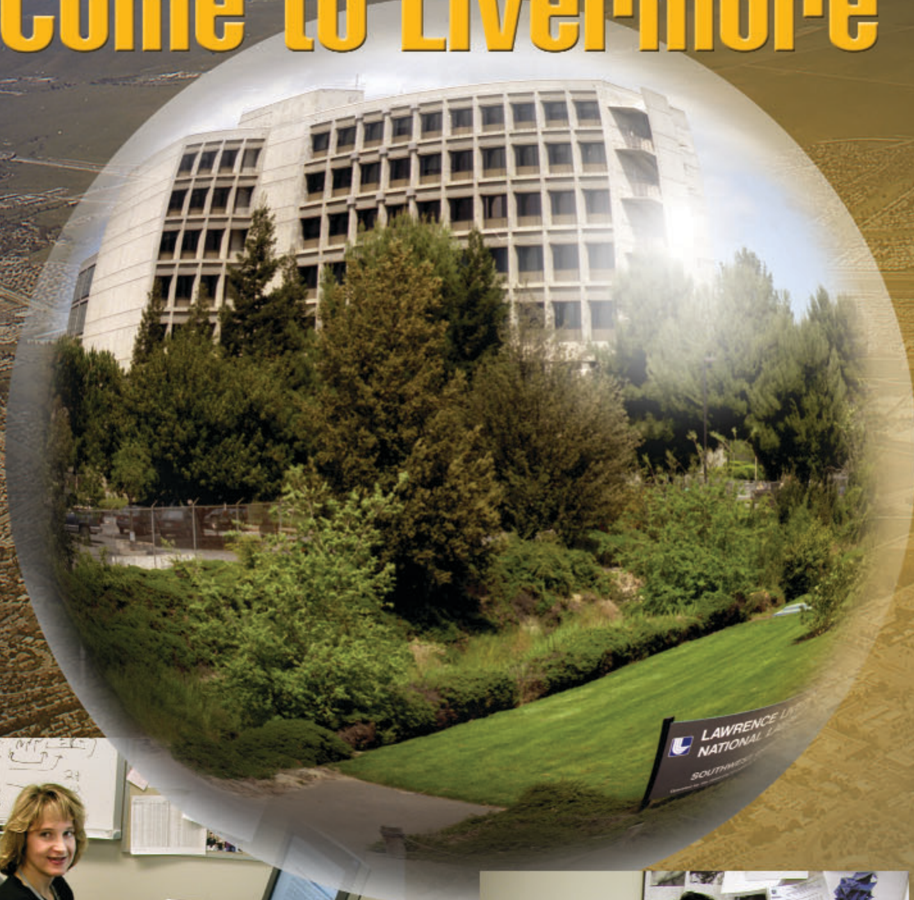
—Arnie Heller

Key Words: Coupled Ocean–Atmosphere Mesoscale Prediction System (COAMPS), fire model, FIRETEC, geographical information systems (GIS), high-gradient flow solver program (HIGRAD), Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, National Atmospheric Release Advisory Center (NARAC), TeraCluster2000 supercomputer, wildfires.

For further information contact Michael Bradley (925) 422-1835 (bradley6@llnl.gov).

The Best and the Brightest Come to Livermore

Fewer than 1 percent of applicants become Lawrence fellows at Livermore.



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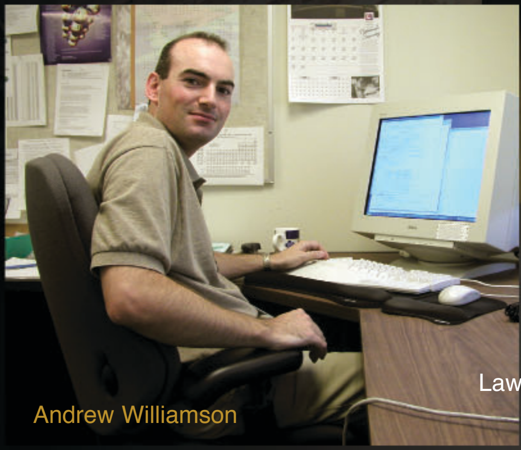


Andrew Williamson

WOULD you apply to be a Lawrence fellow, knowing your chances were less than 1 in 100 of being accepted? For the applicants, the stakes are high. But the payoff is great for both the fellows and the Laboratory.

This postdoctoral program is formally known as the Lawrence Livermore Fellowship Program. Informally, it is called the Lawrence Fellowship in tribute to Ernest O. Lawrence, the cofounder of the Laboratory, who cultivated creativity and intellectual vitality in the scientists who worked with him. Lawrence Livermore National Laboratory strives to do the same.

The Laboratory has always been a place where postdoctoral fellows thrive. They can work on state-of-the-art equipment with leaders in their field, performing research in areas of high demand. While all postdoctoral fellows pursue independent research, most are hired by a particular program, usually to perform research for a specific project. Lawrence fellows have no programmatic responsibilities and are given the opportunity to select the group in which they want to work. The allure of freedom and an atmosphere that cultivates creativity, coupled with a competitive salary and Livermore's extensive resources, make the Lawrence Fellowship Program a prestigious opportunity. In exchange, it brings to Livermore some of the most sought-after Ph.D.s in the world.

The fellows produce remarkably creative research during their tenure. Many stay on as full-time career employees, continuing their work. Some leave Livermore to take positions at other institutions. But, as one fellow says, "The ones who leave are ambassadors for Livermore for the rest of their careers."

Olgica Bakajin

Solution to a Challenge

The Lawrence Fellowship Program was the brainchild of Jeff Wadsworth, former deputy director for Science and Technology. He initiated the program in 1997 in an effort to reverse the effects of the "dot-com" boom, which was leading many young scientists to choose the remuneration offered by private industry over employment with Department of Energy laboratories.

To help persuade the best and the brightest to come to Livermore, the Lawrence Fellowship offers an attractive salary and considerable research freedom. It was modeled after the J. Robert Oppenheimer Postdoctoral Fellowship Program at Los Alamos National Laboratory. In both programs, non-U.S. citizens may apply. Lawrence fellows are hired by the Director's Office, in cooperation with Livermore's University Relations Program.

The new program was first announced in the fall of 1997. Although some Lawrence fellows learn about the program through contacts with Laboratory employees, most applicants find out about it through advertisements in journals such as *Science* and *Nature* or on the Web at either fellowship.llnl.gov/ or www.llnl.gov/postdoc/.

"We are interested in finding people who weren't necessarily thinking about coming to Livermore or who didn't know about Livermore initially," says Harry Radousky, chair of the Lawrence Fellowship Program committee.

The fellows are chosen for 3-year appointments by a selection committee consisting of a representative from each of the Laboratory's scientific directorates. The criteria for acceptance are rigorous. Out of 1,849 applicants in the first 4 years of the program, only 15 have been accepted. More recently, 282 applications were received for the program's fifth year, and 2 applicants have been invited to participate.

Each application is read by the selection committee, which looks primarily for leadership of stellar research projects. Applicants must have received their Ph.D. within the last 5 years. The applicant pool is eventually reduced to 6 individuals who undergo a 2-day interview. On the first day, the fellowship finalist gives a seminar on his or her area of interest; has lunch with the committee, which serves as a question-and-answer session; and then meets with current fellows in the afternoon. On the second day, applicants have the opportunity to talk to Laboratory scientists with whom they might be interested in working.

The goal of this process is to find people who will succeed at the Laboratory. The likelihood of success is measured in several ways: by matching an applicant's field of interest with those of the Laboratory, examining the applicant's academic record and publications, and analyzing the research projects the applicant has initiated and the level of innovation those projects represent.

"We're not looking for management skills but at scientific leadership," says Radousky. "The object of the fellowships is to encourage intellectual vitality at the Lab and to recruit the best people in the world," he continues. "What we've discovered is that the application process is an excellent way to attract people to all kinds of positions. Many applicants who don't get into the Lawrence Fellowship Program are awarded postdoctoral fellowships to work in Laboratory programs or are hired as full-time employees."

Of the 15 individuals who have received Lawrence Fellowships thus far, 3 are now career employees, 2 left to become professors at the Massachusetts Institute of Technology (MIT), 1 went to the National Institute for Standards and Technology, another returned to his native Belgium, and the remaining 8 are still Lawrence fellows.

The Results of Freedom

Freedom to work on projects and with mentors of their choice is what most current Lawrence fellows say attracted them to the program. This freedom, coupled with the Laboratory's interdisciplinary atmosphere, also permits many fellows to move outside their initial area of specialization and investigate other scientific fields.

Wei Cai, for instance, a current Lawrence fellow from China, earned his Ph.D. from MIT. Midway through his graduate work, mentor Vasily Bulatov left MIT for the Laboratory. Bulatov encouraged Cai to apply for the program. Cai was a successful fellowship applicant and has worked not only with Bulatov but also with Malvin Kalos, the father of quantum Monte Carlo simulations. With Kalos,

Julio Camarero

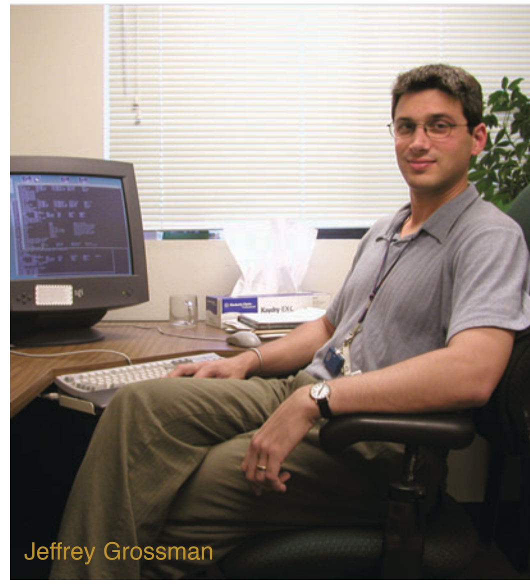
Cai has been investigating how to use Monte Carlo simulation codes more efficiently for modeling the microstructures of materials. Cai has amended some of Kalos's techniques and applied them to small-scale problems with great success. Now, together with Kalos, Bulatov, and other Livermore researchers, Cai is working on a project funded by the Laboratory Directed Research and Development (LDRD) program to apply these techniques to larger, more complex systems. Cai has also been working on a new massively parallel computer code for modeling dislocation dynamics. "What happened here has a lot to do with the academic freedom the fellowship provides," Cai attests.

This freedom also allowed Cai to work on a particularly exciting project far removed from his usual line of research. At the suggestion of Giulia Galli, leader of the Quantum Molecular Dynamics Simulations Group, Cai tried to solve a problem that Galli's group was facing: adding a means of modeling a magnetic field to the electronic structure simulation codes regularly used to model condensed matter systems. Cai devised a code that successfully modeled in two dimensions the behavior of small systems, such as isolated hydrogen atoms and molecules, under an arbitrary magnetic field. The next step will be to apply this method with the more powerful electronic structure codes used for large-scale calculations, such as the modeling of magnetic field effects on the dynamics of fluid hydrogen.

Cai notes that the freedom allowed in the Lawrence Fellowship Program can be almost disconcerting at times. "You need discipline and must be able to make decisions at critical times about what you want to study."

Working at the Nanoscale

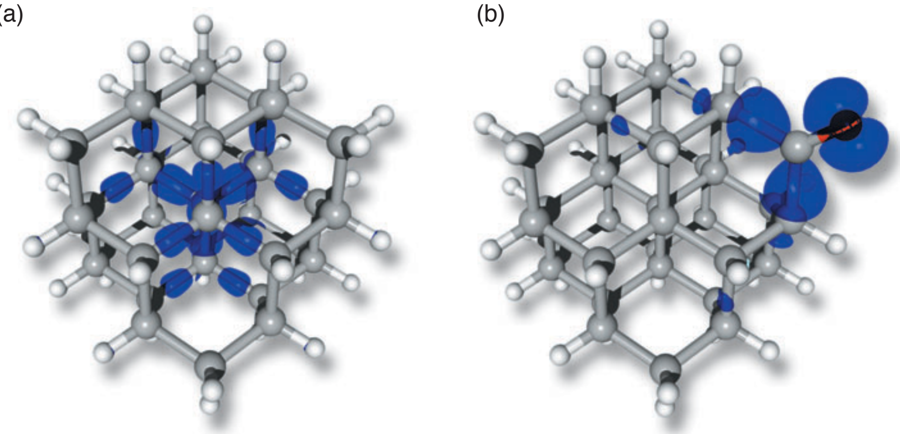
Two computational physicists became a team as Lawrence fellows. Jeffrey Grossman, a Ph.D. from the University of Illinois at Champaign-Urbana, and Andrew Williamson, a Ph.D. from the University of Cambridge in England, had known each other for years and both were interested in working with Giulia Galli. Almost immediately after arriving at Livermore as fellows, they applied for LDRD funding to use quantum Monte Carlo simulations to learn more about the characteristics of nanostructures, atomic-scale dots 1,000 times smaller than the width of a human hair. (See *S&TR*, April 2002, pp. 4–10.)


Jeffrey Grossman

"Scientific interest in nanotechnology centers around one very simple concept," says Grossman. "When you make something really small, its characteristics change. At the nanoscale—just a few hundred atoms—a material's properties start changing and become really interesting. Those differences and the ability to control the size of the structures mean that all kinds of new devices could be made—new ways to deliver drugs, storage systems for hydrogen fuel, detectors that can recognize microscopic amounts of anthrax in the air."

Livermore's supercomputers were a major draw for this duo because quantum Monte Carlo simulations are computationally intensive. With Livermore's computers, they can do

(a) (b)



Lawrence fellows Jeffrey Grossman and Andrew Williamson are using quantum Monte Carlo simulations to research the characteristics of nanostructures such as these silicon quantum dots. (a) A 71-atom silicon quantum dot. Hydrogen atoms (white) bonded to the surface make the material less reactive. (b) When a more reactive oxygen atom replaces two hydrogen atoms, the electron charge cloud (purple) is drawn toward the oxygen atom, dramatically changing the optical properties (wavelength) of the silicon quantum dot.

work that they couldn't do at most places.

Another selling point was that Galli's group was beginning a new project on nanoscience when Grossman and Williamson joined the Laboratory. "Part of what makes the Lawrence Fellowship Program so attractive," says Williamson, "is the opportunity to create something new and shape the direction that research takes, rather than trying to come in and fit into a slot that was shaped by someone else."

Experimental biologist Julio Camarero, who is also working at the nanoscale, saw the Lawrence program advertised in *Science* and *Nature* while a postdoctoral fellow at Rockefeller University in New York City. Camarero received his Ph.D. from the University of Barcelona.

At Livermore, he started out in the Biology and Biotechnology Research Program (BBRP) but moved to the Chemistry and Materials Science Directorate, where he continues to perform biological experiments. He is a member of a team that aims to use dip-pen nanolithography to create and probe ordered arrays of proteins and colloids. One of the many uses for dip-pen nanolithography is to create tiny sensors that will detect biological warfare agents.

"The Lab is interested in applying science and technology to create tools for national security," notes Camarero. "I think that the technology we have developed is very powerful and has many applications, not the least of which is protecting us from biological terrorism."

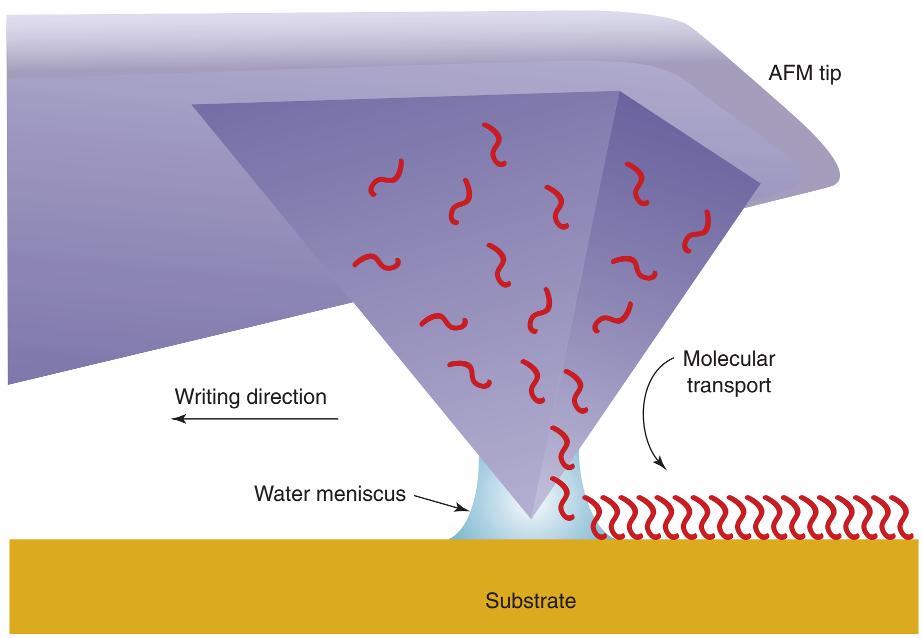
In dip-pen nanolithography, the tip of an atomic force microscope is dipped into either an organic or inorganic substance (the "ink") and then is used to "write" on the surface of an inorganic substrate. (See *S&TR*, December 2001, pp. 12–19.) As the tip moves across the surface, it creates a precise, orderly pattern, or template, of material that is in chemical contrast to the substrate surface.

The goal of Camarero's research is to form specific chemical patterns less than 10 nanometers wide on silicon dioxide and gold surfaces. The chemicals in this template will react with proteins, thus making the template a sort of "molecular Velcro" to which the proteins bind in ordered arrays. Use of these templates allows for total control over the orientation of the proteins.

Small, Complex Systems

Kenneth Kim was at the University of Cambridge as a Wellcome Trust fellow in the Applied Mathematics and Theoretical Physics Department when he learned about the Lawrence Fellowship Program from colleagues at the University of California at Berkeley and from Livermore's Web site. Kim works in BBRP's Computational and Systems Biology Division, led by Michael Colvin. "Traditionally, biology has been a qualitative discipline," Kim says. "But mathematics can play an important role in the biological sciences by providing a precise and powerful language to clarify underlying mechanisms and reveal hidden connections between seemingly disparate systems. Mathematical modeling may allow biology to become a predictive science alongside physics and chemistry."

Kim is applying the mathematical methods of statistical mechanics to the study of the astonishingly complex interactions and collective behavior of biological systems. He has studied the collective behavior of interacting bodies (inclusions) in an elastic medium (a cell membrane). The mathematical model that describes this behavior can be used to investigate the mechanism that causes protein inclusions in cellular membranes



Lawrence fellows Julio Camarero and Aleksandr Noy—now a full-time Laboratory employee—are pursuing research using dip-pen nanolithography. This technology uses the tip of an atomic force microscope (AFM) dipped in molecules to "write" on an inorganic substrate. The molecules react with the substrate to create a pattern of nanostructures attached to the substrate. These nanostructures have a variety of scientific uses.

to distribute themselves into large, stable aggregates as a function of their global shape. This research illustrates the rich interplay between geometry and statistical mechanics that underlies biological and other complex systems.

Kim is also developing a mathematical model for gene regulatory networks. In a gene network, the protein encoded by a gene can regulate the expression of other genes, which in turn control other genes. A protein can also regulate its own level of production through feedback processes.

"This network of interacting genes is another concrete example of collective behavior exhibiting an amazing degree of complexity at many spatial and temporal scales," says Kim.

Olgica Bakajin of Yugoslavia is yet another fellow working at the nanoscale. Bakajin had completed her Ph.D. at Princeton University and was on her way to the National Institutes of Health (NIH) when Livermore called to inform her that she was a successful Lawrence fellow applicant. Since arriving at Livermore, she has worked on several projects related to the development of novel microstructures and nanostructures. She is designing and fabricating a fast microfluidic mixer for the study of proteins. Just 10 micrometers wide—a human hair is 80 micrometers wide—the mixer can cause proteins to fold and unfold when solution conditions in the mixer are changed quickly and precisely. Bakajin will be using the mixer to examine the kinetics of fast protein folding reactions (an LDRD-funded project) and to investigate the kinetics of the folding of single-protein molecules (a collaboration with NIH scientists).

Working with former Lawrence fellow Aleksandr Noy, Bakajin is using carbon nanotubes in microfabricated devices to separate biological molecules. In the future, these microdevices could be used as detectors of chemical and biological warfare agents. "The interdisciplinary atmosphere at the Lab has provided me with lots of research opportunities," says Bakajin. "Right now, I have more ideas for interesting projects than I have time to pursue them."


Robert Heeter

Here to Stay

Three former fellows are now full-time Laboratory employees, having exchanged some of the freedom of the Lawrence Fellowship for a staff position.

Theoretical biologist Shea Gardner, who studied population biology at the University of California at Davis, worked initially on several computational biology projects, one of which was a mathematical model to tailor chemotherapy treatments for individual cancer patients. Treatment strategies are based on the kinetics of the patient's particular tumor cells. Gardner has filed a provisional patent for this modeling approach and has been contacted about commercially developing the software.

Gardner also worked on biostatistics for the analysis of gene microarrays. A microarray is a glass microscope slide covered with "spots," each occupied by a different gene. (See *S&TR*, March 2002, pp. 4–9.) The entire slide is exposed to a stimulus such as a chemical or a change of temperature, and scientists note how each gene responds to the stimulus. "With microarrays, you can see the expression of over 12,000 genes at once, in a single run," Gardner notes. "Previously, you could look at just one gene at a time."

Gardner is now participating in bioinformatics work for the National Nuclear Security Administration's Chemical and Biological National Security Program, computationally identifying DNA signatures that could be used to detect biological pathogens. She hopes to continue with this research. "Mathematical modeling, biostatistics, and bioinformatics are really different," she says. "Where else would I have had the opportunity to work on all three?"

Aleksandr Noy, a physical chemist from Harvard University, came to Livermore in 1998 to work on high-resolution microscopy. To that end, he developed a new microscope system that combines the topographic capabilities of the atomic force microscope with the spectroscopy capabilities of a confocal microscope. (See *S&TR*, December 2001, pp. 12–19.)

"My interests morphed from just looking at tiny things to fabricating them and using them for nanoscience applications," he says. "Shifting focus like that would not have been possible if I had not been a Lawrence fellow." Noy has worked on several nanoscience projects, including some that use carbon nanotubes in unique ways. Much of his research requires his new microscope to make the results visible.

He now leads a group that is fabricating electroluminescent nanostructures by dip-pen nanolithography. The researchers "write" with a conjugated polymer that emits light when a voltage is applied. Nanowires made of conjugated polymer poly [2-methoxy, 5-ethyl [2´ hexy(oxy)] para-prenylene vinylene], or MEH-PPV, may some day serve as light-emitting nanodiodes. MEH-PPV nanowires are also highly sensitive to light and can serve as tiny optoelectric switches, which today are typically 1,000 times larger than tomorrow's MEH-PPV nanowires will be.

Plasma physicist Robert Heeter heard about the Lawrence Fellowship Program from Paul Springer, a group leader in Livermore's Physics and Advanced Technologies Directorate, who performs laboratory astrophysics experiments. Heeter has been working with Springer since coming to Livermore in 1999.

While at Princeton University earning his Ph.D., Heeter worked in England at the Joint European Torus, a magnetic fusion energy facility. But because of funding cuts, magnetic fusion research had fewer opportunities when Heeter was about to graduate. He was also interested in astrophysics, so he decided to apply for a Lawrence Fellowship at Livermore, which had active programs in both astrophysics and fusion energy.

Heeter became a Lawrence fellow and almost immediately got involved in photoionization experiments on Sandia National Laboratories' *Z* Accelerator in Albuquerque, New Mexico. Today, he continues his photoionization research. "I've also been doing other experiments in high-energy-density plasma physics," he adds. "I've stayed in the same group and in the same field that I was in as a fellow. High-energy-density physics experiments have numerous applications: in stockpile stewardship, in inertial fusion, and in astrophysics. And there's a lot of fundamental science to explore that hasn't been done before."

Laboratory Ambassadors

Not all Lawrence fellows stay on as full-time Laboratory employees. The most recent one to depart was metallurgist Christopher Schuh, who left in the summer of 2002 to become a professor at MIT. After completing his Ph.D. at Northwestern University, he came to Livermore to work on grain boundary engineering, in which conventional metallurgical processing is tailored to produce better metals. Grain boundaries—where crystals with different orientations come together—are the weak link in any material. Schuh examined ways to manipulate the orientation of crystals at grain boundaries to create metals with desirable properties such as less cracking, corrosion, and cavitation.

Schuh's research also took him beyond grain boundaries to the individual atoms in the crystals. "If you disturb the atoms in metals so much that the crystal structure no longer looks anything like that of traditional metals, the metals will have very different properties," says Schuh. "We're trying to understand how these changes affect the physics of the metal."

Schuh notes that postdoctoral fellows typically join a program with the understanding that they have been hired to work with someone on a certain project. "For Lawrence fellows," he says, "there's no such obligation. That gives you complete freedom and a lot of latitude."

Nicolas Hadjiconstantinou received his Ph.D. from MIT and immediately


Aleksandr Noy

joined Livermore as a Lawrence fellow, deferring a teaching appointment at MIT for a year. While at Livermore, he helped to develop a code that extended the use of direct Monte Carlo calculation from the simulation of dilute gases to the simulation of dense fluids. With this code, Livermore researchers can simulate for the first time the phase change characteristics of a van der Waals fluid.

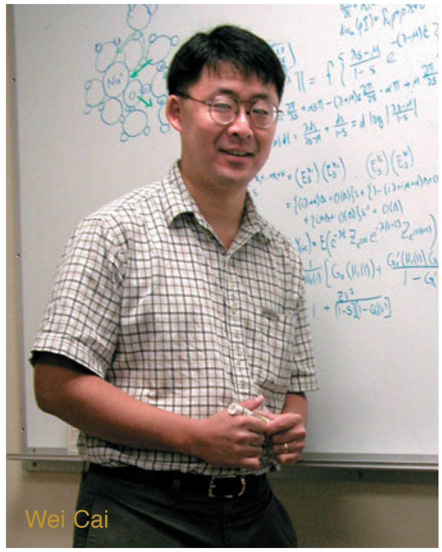
Joel Ullom, who completed his Ph.D. at Harvard, focused on the development of cryogenic detectors, which are small electrical circuits that produce a current or voltage pulse when hit by a photon or particle. The detector

Olgica Bakajin is designing and fabricating this fast microfluidic mixer used for researching the kinetics of protein folding.

must be cooled to temperatures between 0.1 and 1 kelvin, so that the energy of a single photon will produce measurable heating. Ullom used cryogenic detectors to weigh the protein fragments dislodged from bacterial spores by a pulse of laser light. He also developed refrigeration technology to produce the ultralow temperatures needed for cryogenic detectors. Ullom became a Laboratory career employee before leaving for a position at the National Institute of Standards and Technology.

Luc Machiels, a native of Belgium,

One of the research interests Shea Gardner pursued as a Lawrence fellow, which she continues today as a Laboratory employee, is modeling the DNA signatures of viral pathogens. These simulations contribute to technologies for detecting agents of biowarfare.



Wei Cai

received his Ph.D. from the Swiss Federal Institute of Technology. After a postdoctoral position at MIT, he came to the Center for Applied Scientific Computing, where he solved problems in continuum mechanics. With colleagues at MIT, he developed a new finite-element error control strategy for the version of the Navier–Stokes equation that describes the motion of an incompressible fluid. The technique, which is both accurate and efficient, calculates lower and upper limits for the output of a system, such as the temperature bounds at the surface of an electronic device. Before leaving Livermore, he also developed new techniques for the solution and modeling of partial differential equations.

A Resounding Success

Radousky has only good things to say about the Lawrence Fellowship Program. “We’ve learned that we can attract really top people to the Laboratory,” he says. “This program has attracted the best young scientists to the Lab and promoted university collaborations. It is also an excellent way to do general recruiting.”

When the program first started, more fellows were engaged in traditional physics research, while today more are studying biology and nanoscience. This shift is consistent with changes throughout the scientific community. Biological research leaped to the foreground with the success of the Human Genome Project. Many experts predict that the 21st century will be remembered for a revolution in biotechnology and medicine comparable to the advances made during the last century in physics.

Nanoscience is a similarly “hot” research topic. As all kinds of devices in our world become smaller and smaller, nanostructures of all types will find many uses.

All in all, the Lawrence Fellowship Program has been a resounding success in bringing new talent to the Laboratory and encouraging creativity and exciting science.

—Laurie Powers and Katie Walter

Key Words: Lawrence fellows, Lawrence Fellowship Program, postdoctoral positions.

For further information contact Harry Radousky (925) 422-4478 (radousky1@llnl.gov).

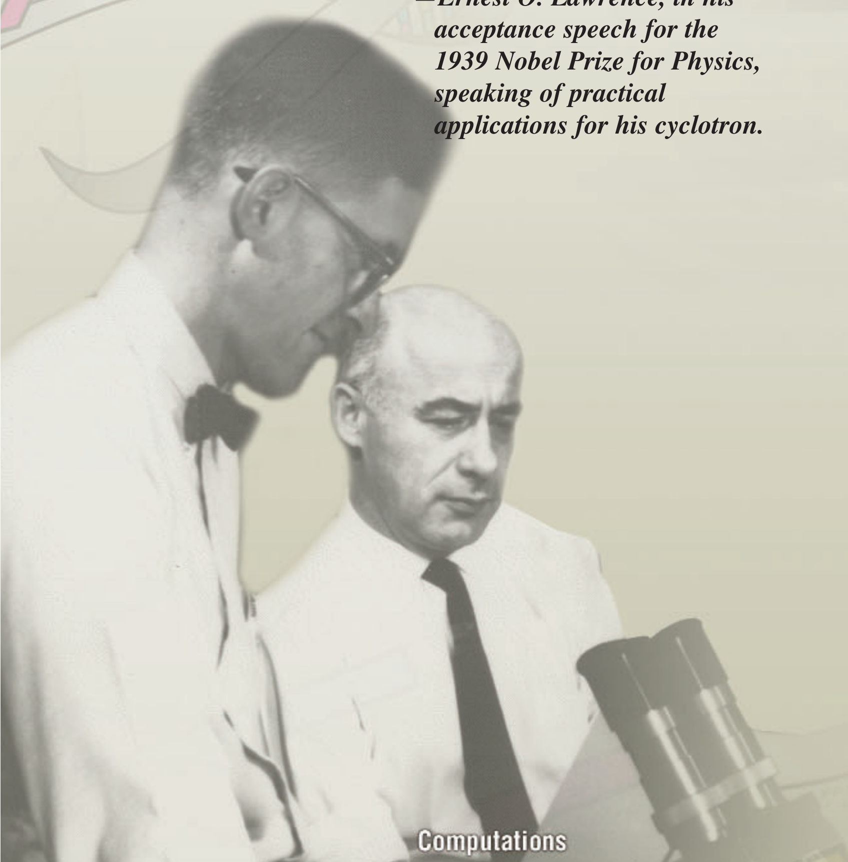
For information on the Lawrence Fellowship Program and other fellowship opportunities at the Laboratory, see these Web sites:

fellowship.llnl.gov/
www.llnl.gov/postdoc/

Biological Research Evolves at Livermore

"We count it as a privilege to do everything we can to assist our medical colleagues in the application of these new tools to the problems of human suffering."

—Ernest O. Lawrence, in his acceptance speech for the 1939 Nobel Prize for Physics, speaking of practical applications for his cyclotron.



As the Laboratory celebrates its 50th anniversary, its biological research program begins its 40th year. Established in May 1963 by the Atomic Energy Commission, the program's original mission was to investigate the effects of ionizing radiation on humans.

Today, Livermore's biological research extends far beyond studying the effects of radiation. A primary emphasis is countering the terrorist threat that grips our nation. The anthrax scares in the fall of 2001 alerted us to the danger of bioterrorism and heightened the need for fast, accurate, inexpensive methods to detect biological warfare agents. Fortunately, long before last fall, Livermore was a leader in developing innovative methods and technologies for early detection of bioterrorism threats. Since the attack, the Laboratory has intensified its efforts in this area so vital to national security.

Radiation effects and bioterrorism response have more in common than might at first be apparent. The link is DNA, the genetic code of all living things. Technologies developed during Livermore's studies of how radiation affects DNA contributed to the founding of the Human Genome Project, the largest biological research project ever undertaken. Since the working draft of the human genome was completed in 2000, the genomes of many other animals and microbes have been sequenced. Sequencing the DNA of bioagent microbes supplies the basis for DNA signatures that are being put to work in new detectors.

Livermore's early analysis of DNA damage has evolved into long-term research in several areas important to human health. Research on radiation exposure resulted in new assays that were first used to evaluate genetic changes in atom bomb survivors in Japan and later applied to understanding the exposures incurred by workers who cleaned up the Chernobyl nuclear power plant after the 1986 accident. Several of these tools have broad application in bioscience. Another research area focuses on how DNA repairs itself. One project analyzes the ways that damaged DNA affects sperm during critical stages of reproduction. Another examines how cooking certain foods produces chemicals that damage DNA. Along the way,

Livermore bioresearchers have pioneered many new tools and methods for bioscience research, often collaborating with physicists, chemists, engineers, and computer scientists.

In 1972, Roger Batzel, then Laboratory director, said, "I personally view Bio-Med as an area which could well grow. It's been a relatively small program, but I think it could develop into one of the strengths of the Laboratory."

Batzel could hardly imagine how dramatically Livermore's nascent biomedical program would grow and change. The recent proposal to establish a homeland security center of excellence at Livermore owes much to the distinguished efforts over the years of many Livermore biological research scientists.

During the 1983 celebration of the 20th anniversary of biomedical research at Livermore, then Laboratory Director Roger Batzel, Associate Director Mort Mendelsohn, and former Program Director John Gofman viewed the work of bioscientist Laurie Gordon.

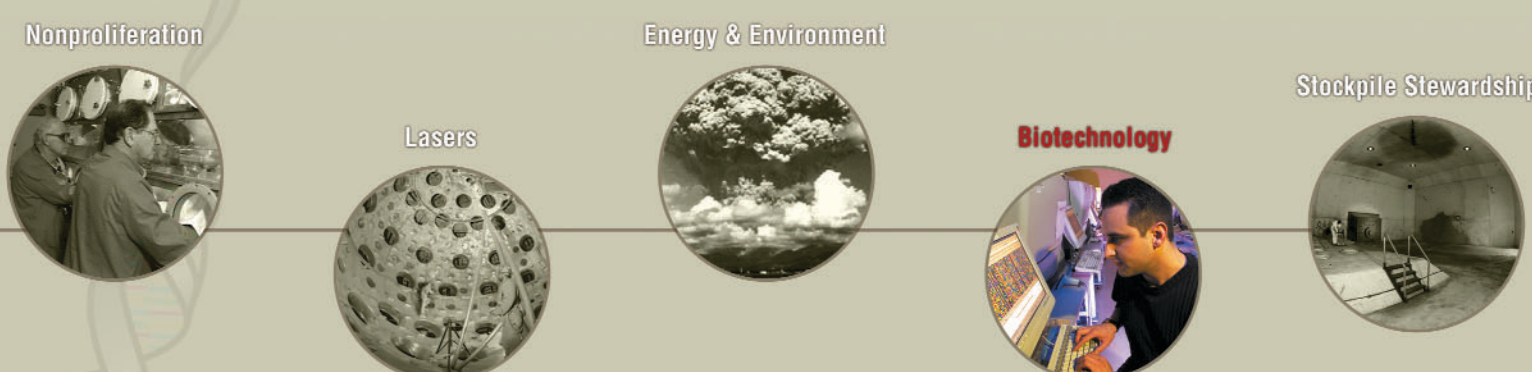
Of Chromosomes and DNA

Biological studies at Livermore have two major origins. One was the advent of thermonuclear testing in the Pacific Ocean during the mid-1950s. The other was Project Plowshare, which was devoted to the peaceful uses of nuclear weapons for stimulating underground natural gas production, mining, blasting out harbors, and perhaps even creating a new Panama Canal. Testing in the Pacific and in the Soviet Union had made radioactive fallout a major public issue. With Plowshare's vision of nuclear explosions near populated areas for routine engineering tasks, nuclear contamination became a more direct concern.

John Gofman, a professor of medical physics at the Donner Laboratory of the University of California at Berkeley, was recruited to set up the new program. As it happened, Project Plowshare was largely shelved by the time Gofman started working. "But he studied the dose to humans anyway, with an emphasis on radiation safety," says Mort Mendelsohn, who followed Gofman as leader of the biomedical research program.

By 1963, the scientific community suspected that DNA was the cellular part most sensitive to radiation damage. Gofman had already become involved in cytogenetics, the study of chromosomes, a field that was making major advances at the time. According to Mendelsohn, "Gofman wanted to measure chromosomes for a reason that was way ahead of its time." Many researchers were growing cancer cells in culture, and Gofman suggested examining the chromosomes in these cells to see what changes they had in common. He developed a method of analyzing chromosomes by measuring their length. It proved to lack adequate sensitivity, but his work set the stage for future cytogenetics progress at Livermore.

In 1974, two years after Mendelsohn's arrival, Livermore scientists made history when they successfully measured and sorted hamster chromosomes using flow cytometry. In humans and other complex organisms, DNA is packaged into chromosomes. Humans have 23 pairs, or 46 total. With flow cytometry, researchers could for the first time automatically



identify and sort individual chromosomes or whole cells for subsequent assessment.

During the 1970s and 1980s, the Laboratory made rapid advances in flow cytometry and was for many years a premier institution for cytometric research. In fact, Mendelsohn and other Livermore scientists founded the Society for Analytic Cytology, now the International Society for Analytic Cytology. The journal *Cytometry*, first issued in 1980, was published from Livermore for many years. More recently, Livermore engineers miniaturized flow cytometry in microfluidic systems that support medical devices and detectors for biological and chemical agents. (See *S&TR*, November 1999, pp. 10–16.)

By 1979, scientists had learned how to sort human chromosomes, which are much smaller and more varied than the hamster's. By 1984, says Mendelsohn, "We had increased our proficiency and confidence in flow cytometry such that we could separately identify and study each of the human chromosomes." This ability, combined with worldwide developments in recombinant DNA technology, led to the Livermore–Los Alamos project to build human chromosome-specific DNA libraries.

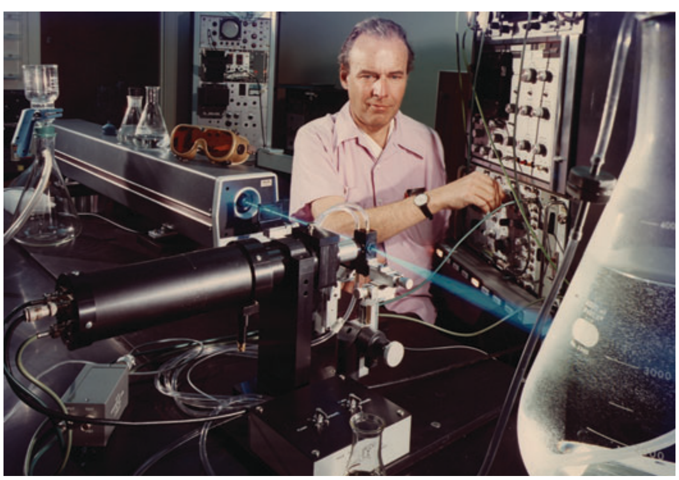
"The development of chromosome-specific libraries was important," continues Mendelsohn. "At that time, sequencing technology was slow and primitive. The thought of sequencing the entire human DNA was overwhelming. But when the sequencing process could be broken down into smaller pieces—chromosomes—it became a possibility."

At a 1984 meeting, molecular geneticists from around the world brainstormed the potential for DNA-oriented methods to detect heritable mutations in the children of people who survived the atom bombs in Japan. Many of the questions were so challenging that large-scale, detailed genomic sequence analysis would be needed to even attempt to answer them. (To this day, the basic question of how often heritable mutations occur remains unanswered.) Recognizing the classes of problems that require large-scale, detailed sequence data helped inspire the idea of sequencing the entire human genome.

In 1986, the Department of Energy launched a major initiative to completely decipher the human genetic code. A year later, Livermore researchers began to study chromosome 19, which they had earlier learned was home to several genes important for DNA repair. DOE joined forces with the National Institutes of Health in 1990 to kick off the Human Genome Project.

In 1992, Anthony Carrano became associate director of biomedical research. Carrano, who had been studying chromosomes and DNA since arriving at Livermore in 1973, was instrumental in building the Laboratory's human genome efforts, particularly sequencing. In 1996, he helped form the Joint Genome Institute (JGI). This collaboration of the Livermore, Berkeley, and Los Alamos national laboratories pooled resources to form a production facility to sequence human chromosomes 5, 16, and 19 for the international Human Genome Project.

During the 1990s, sequencing technologies matured, becoming ever more automated. Sequencing speed increased rapidly. A working draft of the three chromosomes was completed in April 2000, a year ahead of a greatly accelerated



Marv Van Dilla, an expert in flow cytometry, came to Livermore from Los Alamos in 1972. Shown here in 1973, Van Dilla was instrumental in establishing the Laboratory's preeminence in cytometric research. Livermore was the first to use flow cytometry to sort chromosomes.

Bioscientists Anthony Carrano, who later became associate director, and Larry Thompson in 1978. They had just developed a quick and efficient test to detect damage to genes. The test was based on a finding by Livermore scientists that there is a direct relationship between hard-to-spot gene mutations and an easily recognized process that occurs during cell division. Today, Thompson performs research on DNA repair processes.

schedule set just 18 months earlier. (See *S&TR*, April 2000, pp. 4–11.) This accomplishment was a major step toward understanding DNA and its functions and a significant contribution to the completion of draft sequences of the entire genome in June 2000.

Still Much to Learn

In the excitement over the completed sequence of the human genome, it is easy to forget that this step is just a prologue. The next step is to identify all of our genes and determine what they do and how they do it. Comparative genomics—in which the genomes of different species are compared—is helpful. Mouse DNA is useful because about 99 percent of a mouse's genes are similar to human genes. Comparing how these genes work in mice and how they are activated under different conditions tells us much about our own genes. A JGI team led by Livermore biologist Lisa Stubbs compared human chromosome 19 with similar sections of the mouse DNA to understand the functional significance of DNA sequences. (See *S&TR*, May 2001, pp. 12–20.) Stubbs notes, "Imagine taking human chromosomes, shattering them into pieces of varying lengths, and putting them back together in a different order. That's what mouse chromosomes look like." The Japanese pufferfish (fugu) has also been sequenced because its genome is a compact version of our own.

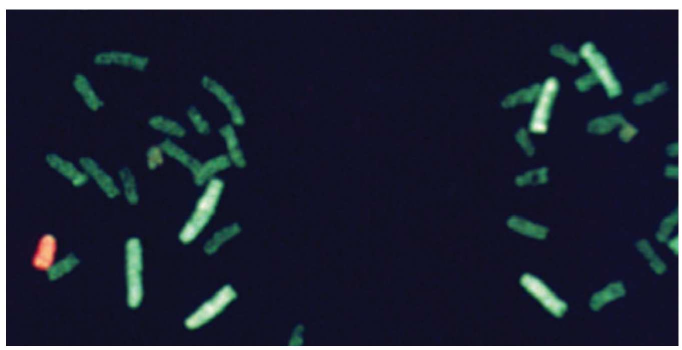
Another outgrowth of the Human Genome Project is proteomics, the study of the 100,000 or so proteins that are generated by our DNA. Proteins are the building blocks of our cells and of the molecular machinery that runs our tissues, organs, and bodies. Understanding how proteins operate is essential to understanding how biological systems work.

X-ray crystallography and nuclear magnetic resonance spectroscopy are two tools Livermore is using to determine the three-dimensional structure of proteins at the atomic level. From that structure, computational methods can attempt to model a protein's function. But determining the structure protein by protein would take years of research to complete. Instead, Livermore scientists are using the minimal data available in computational models to try to predict a protein's structure.

Measuring Radiation Effects

In the first 10 years of Livermore's biological research program, scientists searched for biological measurements that would indicate the radiological dose to which an individual had been exposed. Livermore developed several biological dosimeters to detect and measure changes in human cells,

Researcher Laura Chittenden is shown with a mouse. Mouse DNA, 99 percent of which is similar to human DNA, is being compared to human DNA to help uncover clues to gene regulation and control.



Chromosome painting is the process scientists use to fluorescently label small pieces of DNA from a chromosome-specific library. These chromosome-specific fluorescent probes bind to complementary sequences of the target chromosome and, when viewed under a microscope using fluorescent light, can reveal a targeted gene along a chromosome. This photo is of chromosomes from one-day-old mouse embryos. The bright green chromosomes are chromosomes 1, 2, 3, and X. The orange one is chromosome Y.

significantly advancing the study of human radiation biology and toxicology. The first was the glycophorin-A assay that detects residual mutations in human red blood cells from exposure to radiation decades earlier. Its first use was on atom bomb survivors in Japan.

Work on the glycophorin-A assay begat one of Livermore's first biotechnology projects. In the late 1970s, Laboratory biologists needed antibodies that recognize the subtle distinction between normal and mutant red blood cells. Researchers rolled up their sleeves and began to produce these and many other made-to-order monoclonal antibodies (antibodies derived from a single cell) with a range of potential uses—from detecting sickle cell anemia to evaluating how fast cancer cells are growing. Livermore is no longer in the production mode, but many of its monoclonal antibodies were commercially produced and used by others.

Another important technology developed at Livermore in the mid-1980s is chromosome painting. Scientist Dan Pinkel was instrumental in developing this technology, and the patent for this work has been one of the most lucrative in Livermore's patent portfolio for the past several years.

When first developed, chromosome painting was used to identify DNA damage in which the ends of two chromosomes break off and trade places with each other. These "reciprocal translocations" are one of the distinguishing effects of radiation damage to DNA. Using chromosome painting, scientists can see and count translocations between two differently painted chromosomes to determine a person's likely prior exposure to ionizing radiation. This method of identifying translocations is 10 to 100 times faster than it was before, with greatly increased reliability.

Biology Meets the Computer—The Early Days

Throughout its 50-year history, the Laboratory has pioneered the use of powerful computers to solve complex scientific problems. Challenges in biological research were no exception.

In the mid-1960s, new work on the dynamics of cell multiplication made use of computer codes first developed for Livermore's weapons program. Part of an effort to design an optimal radiation dosage program for cancer therapy, the study included an ingenious calculation system using computer codes to simulate cell activity.

A remarkable combination of an electron microscope and a computer in 1968 produced dramatic three-dimensional images of organelles, tiny working parts within the cell nucleus. Using essentially the same process the human brain uses to produce three-dimensional images from two flat pictures—one taken with each eye—the computer took 12 electron microscope shots, integrated the information, and created three-dimensional images of the organelles that were 50,000 times their real size. The feat had never before been accomplished.

By 1973, Livermore's cytophotometric data conversion system (CYDAC) was attracting interest when it showed that it could measure the DNA in individual chromosomes to great sensitivity. CYDAC studies showed unsuspected small differences in chromosomal DNA content among supposedly normal individuals.

In its first clinical application in 1974, CYDAC confirmed a suspected chromosome abnormality in a patient with chronic myelogenous leukemia (CML). In the early 1960s, scientists discovered that CML was invariably associated with a loss of genetic material from a portion of chromosome 22. This aberration was rarely found otherwise. About 10 years later, researchers at the University of Chicago found an excess of chromosomal matter on chromosome 9 in the same patients. They suspected that the lost material from chromosome 22 had been captured by chromosome 9. It took CYDAC's unprecedented precision to confirm that hypothesis and set cancer researchers on the track of other DNA translocations.

Bioengineers at Livermore combined mechanical skills with an understanding of biology to design the cytophotometric data converter (CYDAC), a highly sensitive diagnostic instrument that measures the amount of DNA in chromosomes. In this 1976 photograph, bioresearcher Linda Ashworth uses CYDAC to scan chromosomes from a mammalian cell.

A third dosimetry method measures the frequency of mutations in the hypoxanthine phosphoribosylantransferase (HPRT) gene in lymphocytes. This assay was developed elsewhere, but since the 1980s, researchers led by biological scientist Irene Jones have greatly expanded understanding of the assay's ability to detect DNA damage from ionizing radiation.

Immediately after the 1986 Chernobyl nuclear accident, the glycophorin-A assay was put to work to screen cleanup workers for their exposures. Years later, bioscientists used the HPRT assay and chromosome painting to measure mutations and alterations in lymphocytes to reconstruct the doses received. (See *S&TR*, September 1999, pp. 12–15.)

To Your Health

A natural extension of studying the effects of ionizing radiation on humans was to explore how radiation and chemicals interact with human genetic material to produce cancers, mutations, and other adverse effects.

In the face of damaging toxins, DNA is able to repair itself—up to a point. How DNA repairs itself has been a focus of ongoing research under bioscientist Larry Thompson almost since the Laboratory began to study DNA damage. Livermore chose to sequence chromosome 19 as part of the Human Genome Project because its properties suggested that it was gene-rich, which proved to be an accurate prediction. Chromosome 19 has the highest gene density of any human chromosome. It was also an apt choice because Livermore researchers had earlier discovered that three genes on chromosome 19 are involved in the repair of DNA damaged by radiation or chemicals. In studies of the Chernobyl cleanup workers, a goal has been to understand why the same dose of radiation has different effects on the cells of individuals. Identifying the differences in DNA repair gene sequence and function for different individuals is key.

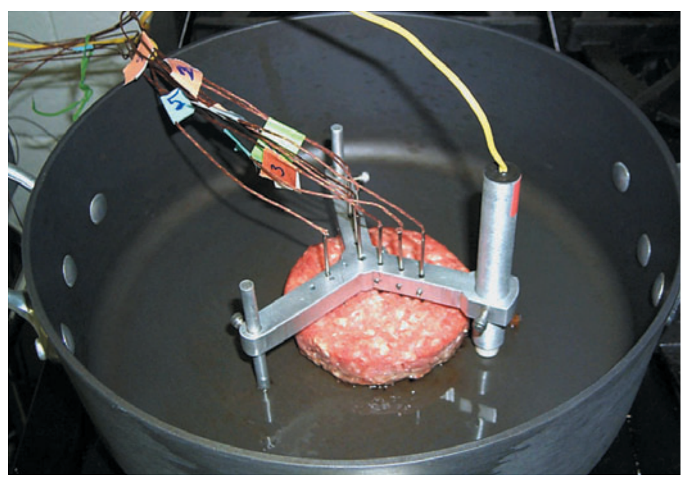
In the 1970s, Livermore's growing expertise in flow cytometry enabled researchers to analyze and sort sperm for the first time. Using this approach, scientists could begin to study the effects of pollutants on DNA during critical stages of sperm formation. Under the leadership of biophysicist Andrew Wyrobek, Livermore has developed several powerful molecular methods to visualize individual chromosomes in sperm and to detect genetic defects in embryos. (See *S&TR*, November/December 1995, pp. 6–19.) These research methods, combined with animal models, have broad implications for screening males for chromosomal abnormalities and genetic diseases, for studying the effects of exposure to mutagenic agents, and for assessing genetic risks to embryos and offspring.

Even the food we eat can damage our DNA. Both 2-amino-1-methyl-6-phenylimidazo [4,5-b] pyrinidine (PhIP) and 2-amino-3,8-dimethylimidazol [4,5-f] quinoxaline (MeIQx) are heterocyclic aromatic amines that appear in meat when it is cooked at high temperature. These compounds and others produced when they are digested form adducts, which are molecules that attach to DNA strands and may interfere with their function. Jim Felton, who is now deputy associate director for Biology and Biotechnology Research Program (BBRP), led a group studying food mutagens for almost two decades.

PhIP and MeIQx have been shown to cause cancer in laboratory animals when administered at high doses. More recently, researchers wanted to know whether DNA and protein adducts can be detected in laboratory animals and humans when they take in a smaller, more typical dietary amount of these substances. In numerous experiments using carbon-14-tagged PhIP and MeIQx molecules, the team has confirmed not only that adducts can be detected at low doses, but also that humans may be more sensitive to these substances than mice or rats.

Such experiments would not have been possible without Livermore's Center for Accelerated Mass Spectrometry. Physics-based accelerator mass spectrometry (AMS) is so sensitive that it can find one carbon-14 atom among a quadrillion other carbon atoms. It can observe the interaction of mutagens with DNA in the first step in carcinogenesis. Livermore is one of just a few institutions in the world using AMS routinely for biomedical and pharmaceutical applications, and it is a recognized leader in the field. (See *S&TR*, July/August 2000, pp. 12–19.)

Continuing a long tradition of collaboration with universities, Livermore joined forces with the University of California at Davis Cancer Center in October 2000 to fight



Meat cooked at high temperatures produces mutagens, which are compounds that can damage DNA. Here, a fully instrumented hamburger patty is fried to determine its temperature as a function of depth as well as the corresponding concentrations of food mutagens. The data are used to develop computer simulations of the cooking process and to predict the formation of mutagens.

cancer, the nation's second leading killer. Together, they are researching cancer biology, prevention, and control as well as new cancer detection and treatment techniques. In July 2002, the center attained National Cancer Center status from the National Cancer Institute. AMS is a key technology in this collaboration's research.

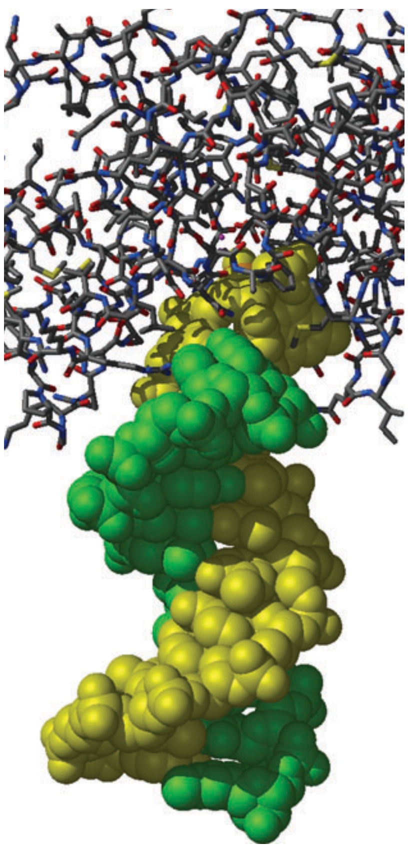
Putting the Computer to Work

Computers have played an integral role in biological research at Livermore for years (see the box on p. 26). In fact, the biomedical program was the first one at Livermore to purchase a personal computer for scientific use. The Procurement Department looked on this purchase with considerable suspicion, viewing a personal computer only as a means to play "Pong." But that little PC automated what had been a tedious manual cell-counting process, and it is impossible to imagine the Laboratory without desktop computers today.

Using both mainframe and personal computers, the Laboratory has pioneered many new ways to use the computer in a biological research setting. Bioinformatics is an area of special strength. In bioinformatics, computer scientists organize the results of molecular biologists' work, developing databases and new analytical tools so that the data can be put to good use. Livermore's leading role in the Human Genome Project would not have been possible without the efforts of BBRP's bioinformatics team. Computer scientist Tom Slezak started this group almost 25 years ago and still leads it.

"Our work is 'bottom of the iceberg' stuff and invisible to most people," says Slezak. "But it's really important. In sequencing the human genome, the flood of data was enormous. As other organisms are sequenced and as the field of comparative genomics takes off, we try to leverage our computational capabilities to stay a step or two ahead."

Computational biology, a relatively recent research area, builds on the Laboratory's strength in computations. According to Michael Colvin, who leads the Computational Biology Group at Livermore, "The emerging explanation of biological functions in terms of their underlying chemical processes is creating an important role for predictive chemical simulations in biological research."



This classical molecular dynamics simulation examines the motion of 1 of 10 proteins of *Escherichia coli* polymerase III, the major DNA replication enzyme in *E. coli* bacteria. This protein's function is to "proofread" a newly synthesized DNA strand by excising any incorrect bases immediately after they are added to the DNA. The goal of this simulation is to understand the chemical mechanism of the proofreading function. Shown as sticks is the proofreading protein. The yellow and green spheres simulate the double-stranded DNA being proofread.

The Handheld Advanced Nucleic Acid Analyzer can detect biological pathogens in the field. It examines the DNA of a sample and compares it with the known DNA sequence of various pathogens such as anthrax and plague. Rapid detection of agents of biological warfare could help save lives because the diseases resulting from many such pathogens are highly treatable if detected early.

Livermore scientists are at the forefront of integrating computation and experiment in bioscience. Ongoing computational biology projects include studying the action of anticancer drugs, DNA-binding properties of mutagens in food, the binding of ligands to selected sites on proteins, the mechanisms of DNA repair enzymes, and the biophysics of DNA base pairing. (See *S&TR*, April 2001, pp. 4–11.)

A particularly exciting tool in computational biology is first-principles quantum mechanics methods to describe the electronic structure of atoms and their chemical properties. Computerized quantum simulations permit researchers to "see" inside biochemical processes to learn how reactions are taking place on a molecular and even atomic level. Such simulations are highly intensive computationally and had to await the arrival of massively parallel computers before they could be performed. (See *S&TR*, April 2002, pp. 4–10.)

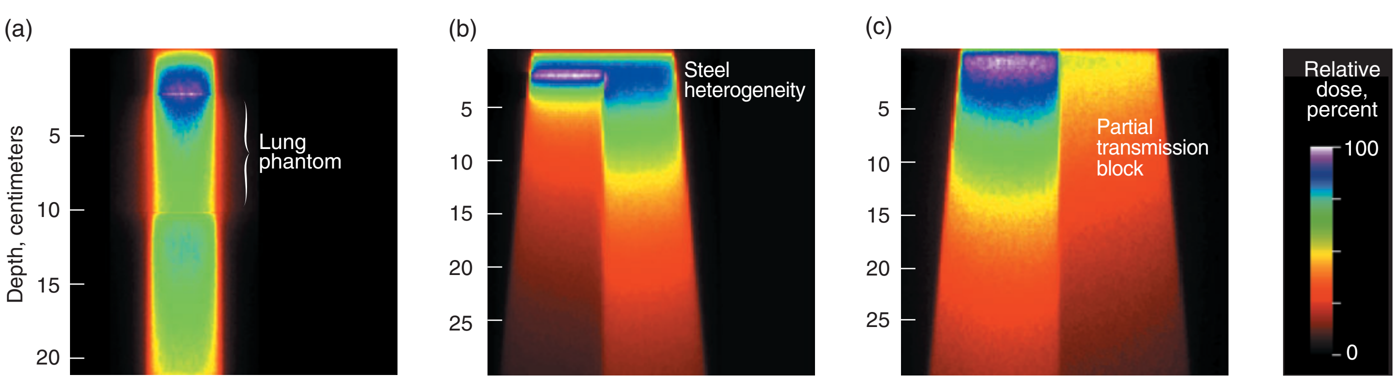
Fighting Bioterrorism

Bacteria, viruses, biological toxins, or genetically altered organisms could be used to threaten urban populations, destroy livestock, and wipe out crops. These agents are difficult to detect and to identify quickly and reliably. Yet, early detection and identification are crucial for minimizing their potentially catastrophic human and economic cost. At Livermore, developing technologies to detect agents of biological warfare has been under way for a decade. Livermore researchers pioneered technologies for rapid detection of tiny amounts of DNA. Equally important has been identifying specific DNA sequences that can be targeted with our detectors. With the recent anthrax attacks and the resulting awareness of bioterrorism threats, Livermore has stepped up its efforts to optimize stationary and portable equipment to detect biological agents.

The foundation for this research was laid during the early years of the program and studies of DNA. For example, by computationally comparing the DNA sequence of *Yersinia pestis*, the bacterium that causes bubonic plague, with the sequence of its close relatives and other bacteria, Livermore has been able to develop unique DNA signatures that allow *Yersinia* to be quickly detected. (See *S&TR*, May 2000, pp. 4–12.)

An entirely new sequencing analysis technique, developed by Livermore's bioinformatics team, recently won one of two 2002 Lawrence Livermore Science and Technology Awards. Using their experience from many years on the Human Genome Project, the team members found a novel way to perform whole genome analysis to compare genomic sequences. With it, they can rapidly determine unique DNA signatures of biowarfare pathogens. They are the first to apply whole genome analysis to pathogens.

Several DNA-detection technologies have been licensed to industry, most recently the Handheld Advanced Nucleic Acid Analyzer (HANAA). Some of these devices depend not only on accurate DNA signatures but also on microfluidics—the miniaturization of piping systems through which fluids flow. In a collaboration with Los Alamos National Laboratory, Livermore's DNA analysis capabilities were used to develop the analysis core of the Biological Aerosol Sentry and Information System, which was deployed at the 2002 Winter Olympics in Salt Lake City, Utah.



PEREGRINE is an innovative radiation planning technology developed at Livermore. Taken by the staff at the University of California at San Francisco, these images of PEREGRINE measurements demonstrate how effectively PEREGRINE can handle different materials and shapes, including (a) heterogeneous materials such as soft tissue and air in the lung, (b) a steel prosthesis, and (c) a partial transmission block that protects healthy tissue from radiation treatment.

Another technique for detecting biological agents focuses on detecting the proteins that DNA generates. Protein detection techniques are typically fast and easy to use but are not as sensitive and specific as DNA detection methods. Livermore is designing seek-and-destroy, antibodylike molecules, called high-affinity ligands, that target specific proteins in biological agents. The development of ligands for detecting tetanus toxin is almost complete. This detection methodology promises to be fast and easy to use as well as highly sensitive and specific. (See *S&TR*, June 2002, pp. 4–11.)

Physics to Biology

Many threads link physics advances and bioresearch progress. Ernest O. Lawrence, founder of the Laboratory, set the precedent for applying tools developed in the course of physics research to fighting human disease. After Lawrence built the cyclotron, he put it to use as a medical tool as quickly as he could. In 1937, Lawrence's mother Gunda was told by many specialists that she had an inoperable tumor. But her life was saved by radiation treatment with the only megavolt x rays then available in the world, using a device developed by her son. She was still living in Berkeley when he died 21 years later.

In this tradition, Livermore recently developed an innovative tool for analyzing and planning radiation treatment for tumors. In the early 1990s, researchers began combining Livermore's huge storehouse of data on nuclear science and radiation transport with Monte Carlo statistical techniques. The result was PEREGRINE, a radiation planning technology that has been licensed to a private company and was approved for use by the U.S. Food and Drug Administration in September 2000. (See *S&TR*, June 2001, pp. 24–25.)

Mrs. Lawrence's treatment and PEREGRINE bring the results of physics research to bear on a pressing medical challenge. Weapons materials have also been used in artificial hip joints designed at Livermore. X-ray tomography developed to examine the inner components of nuclear weapons has revealed the bone weakening of osteoporosis. Quantum simulations, a physics tool that can describe the fundamental interactions of weapons materials, are exposing the inner workings of biochemical processes important to human health. X-ray diffraction using synchrotron light sources, another physics tool, illuminates proteins to help define their function.

The next step in biological research will depend on another tool made possible by advanced physics research—even more powerful computers than are available today. "Where we're going next," says Bert Weinstein, acting associate director for BBRP, "is to understand the whole system of genes. Not just genes as individual parts but as an integrated, intermeshed set of molecular machines, working together to produce the miracle of life."

—Katie Walter

Key Words: accelerator mass spectrometry (AMS), biological warfare agent detectors, chromosome painting, comparative genomics, computational biology, DNA repair, dosimetry, flow cytometry, food mutagens, glycophorin-A assay, Human Genome Project, Joint Genome Institute (JGI), PEREGRINE, proteomics, sperm mutations.

For more information about Biology and Biotechnology Research Program Directorate:
www-bio.llnl.gov/

For details about the history of biology research at Livermore:
www-bbrp.llnl.gov/50_year_anniversary/

For frther information about the Laboratory's 50th anniversary celebrations:
www.llnl.gov/50th_anniv/

Emerging from the Cold War

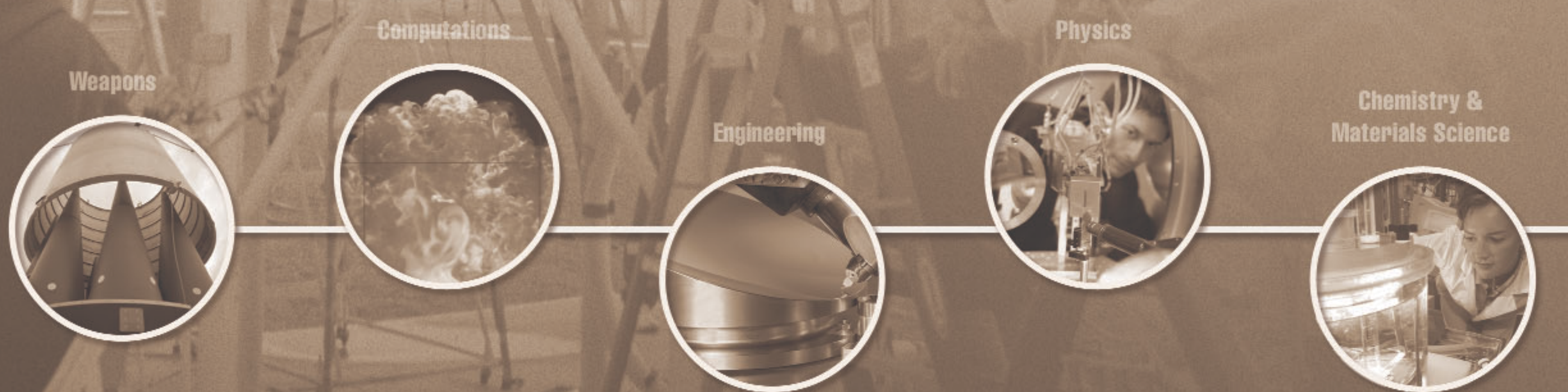
Stockpile Stewardship and Beyond

HISTORIES of the 20th century often celebrate the American spirit that united the country in 1941 after the bombing of Pearl Harbor. The heroism and sacrifice of U.S. citizens, whether fighting on the front lines, building equipment for the military, or rationing supplies at home, marked a great era for this country.

World War II was also a watershed for science and technology research in the United States. Before that war, most scientific research was funded privately. In the 1930s, Ernest O. Lawrence, who later cofounded Lawrence Livermore, built the Crocker Laboratory for housing his fourth cyclotron with contributions from several foundations and individuals, including $75,000 from William Crocker, chairman of the University of California's Board of Regents. But in 1942, the U.S. government found its military ill-equipped for the kind of war it was entering. To bring the military up to date, the government funded an extensive science and technology effort, including the Manhattan Project—a top-secret project in Los

"The science of today is the technology of tomorrow."

—Edward Teller



Alamos, New Mexico, to build the world's first atom bomb.

Reviewing the successes from the war-related research and development effort, President Franklin Roosevelt wrote in a letter to Vannevar Bush, director of the Office of Scientific Research and Development, that the lessons learned by the teams conducting this research could be applied after the war "for the improvement of the national health, the creation of new enterprises bringing new jobs, and the betterment of the national living standard." President Roosevelt asked Bush to recommend a new model for research and development that built on the achievements of the war effort.

In July 1945, Bush presented his recommendations to Roosevelt's successor, President Harry Truman, in a report titled *Science: The Endless Frontier*. The ideas presented in the Bush report shaped research and development activities for the remainder of the 20th century. In particular, government funding for research in support of national security increased dramatically, and improved designs for nuclear weapons continued to be developed at Los Alamos.

After the Soviet Union successfully tested its first atom bomb, the government responded by expanding nuclear weapons research. On September 2, 1952, a branch of the University of California Radiation Laboratory was opened at the deactivated Naval Air Station in Livermore, California.

"The founding of our Laboratory was a realization of the Vannevar Bush model," says physicist Kimberly Budil, who is the current scientific editor for *Science & Technology Review*. "Bush's report recommended that military research continue after the war, so the country would never again have to struggle to catch up technologically in a time of crisis. Also, to support industrial research plus help the economy and improve the American standard of living, the federal government was encouraged to fund basic research and provide educational opportunities—especially to returning soldiers—so the U.S. could renew its talent pool for future science and technology efforts."

The focus of the Laboratory in its early history was on meeting national needs for nuclear expertise. Experts in chemistry, physics, and engineering were encouraged to explore innovative solutions to the problems they faced in developing new weapon designs. Over time, not only did Lawrence Livermore achieve notable successes in its national security mission, but it also became one of the world's premier scientific centers—using its knowledge of nuclear science and engineering to break new ground in magnetic and laser fusion energy, nonnuclear energy, biomedicine, and environmental science.

Budil says that reviewing Livermore's history has given her a new appreciation for its founders. "In 1952, many of the first scientists who joined the Laboratory were young, especially to be taking on this kind of challenge. Herbert York was only 32 years old when he became the first director. The relative youth of our founders, along with their enthusiasm for a new challenge, drove the innovative spirit that we see throughout the Laboratory's history."

Innovative Solutions to Complex Problems

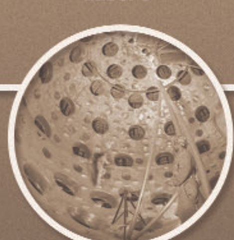
Innovation has been an integral part of Livermore's success. The military requirements for high-yield, low-weight weapons often led researchers to explore new design approaches. For example, in a 1950s project to design a warhead for the Navy's Polaris missile, the Laboratory's goal was to develop a small, efficient thermonuclear weapon that could be carried by submarine. Researchers came up with novel designs for the primary and secondary stages of the weapon to minimize the overall mass of the warhead.

These design improvements had far-reaching effects on future weapon designs. In Edward Teller's autobiography, *Memoirs: A Twentieth-Century Journey in Science and Politics*, he says that the warheads for Polaris greatly improved the nation's ability to deter attack. "That a portion of our retaliatory force would survive a surprise attack guaranteed that the Soviets would never find it advantageous to attempt a first strike."

The success of Polaris also set the tone for research at the Laboratory. Says Budil, "Part of our culture at the Laboratory is a willingness to explore creative solutions so we can find the best approach to the complex issues we need to resolve. That philosophy comes with enormous risk, both for the institution and for individual scientists, but it also offers the

Nonproliferation

Lasers



Energy & Environment

Biotechnology

Stockpile Stewardship

potential for enormous gain. Our history is filled with examples of scientists putting their credibility on the line, risking failure in search of the best solution."

Livermore's multidisciplinary approach to problem-solving was bolstered by the work of scientists and engineers on progressively more complex weapon designs. Because designing a nuclear weapon is an iterative process, weapon researchers often found they had to understand concepts and processes outside their assigned disciplines or areas of expertise.

Test launches of three missiles with Livermore-designed warheads. (a) The Minuteman III intercontinental ballistic missile (ICBM) is equipped to carry the W62 warhead, and (b) the Peacekeeper ICBM is equipped to carry the W87 warhead. (c) The W84 warhead, now inactive, was designed for the ground-launched cruise missile.

For example, at the beginning of a weapons project, computer simulations were often used to evaluate design options. Then, once a new design was built, it had to be tested to ensure it worked as predicted. To acquire data on weapon performance, Laboratory engineers developed diagnostic equipment and techniques that would operate in the highly volatile environment of nuclear tests. These diagnostics had to record data in a fraction of a second, before the detonation vaporized the detectors, test apparatus, and cables.

In developing the elaborate setup for underground nuclear experiments, everyone involved in a test—engineers, physicists, code developers—had to understand the requirements of the other disciplines. According to Laboratory Director Michael Anastasio, this working relationship fostered an integral program of testing, simulation, and fundamental science. "Our work groups had those same permeable boundaries," he says, "where scientists from computation, design, and experimental science all contributed to achieving the goal of delivering a new device."

This multidisciplinary approach to research has provided added benefits to the nation's science and technology base—an advantage Vannevar Bush might have predicted. "To solve the problems encountered in designing nuclear weapons," says Budil, "Laboratory scientists often find themselves at the forefront of new technology. As a result, Livermore has an amazing history of technological firsts as well as spinoff applications that have benefits outside our national security mission."

For example, Livermore developed increasingly powerful lasers—Janus in 1975, Shiva in 1977, and Nova in 1984—so scientists could study thermonuclear physics in a laboratory setting. Data from laser experiments improved computer modeling capabilities for weapons research and were a valuable supplement to underground nuclear tests. But the benefits of laser science and technology extend well past the nuclear weapon community. Programs in inertial confinement fusion and laser isotope separation were begun as efforts to enhance the nation's energy supplies. Other laser research activities set the stage for improving medical treatments and studying the solar system.

"Such advances in scientific understanding and technology development do not happen merely by chance," says Budil. "They require strong capabilities for basic and applied scientific research. Livermore has stable funding, excellent research facilities, and outstanding researchers—factors that are essential to the success of big multidisciplinary science projects. They've contributed to the Laboratory's success both in weapons research and in other programs such as biotechnology and environmental restoration."

A New Course for Weapons Research

Nearly four decades after Lawrence Livermore was founded, the Berlin Wall was torn down, and the Soviet Union collapsed—the Cold War had been won. Today, the U.S. maintains a much smaller stockpile of weapons, but nuclear deterrence remains an integral part of its national security policy.

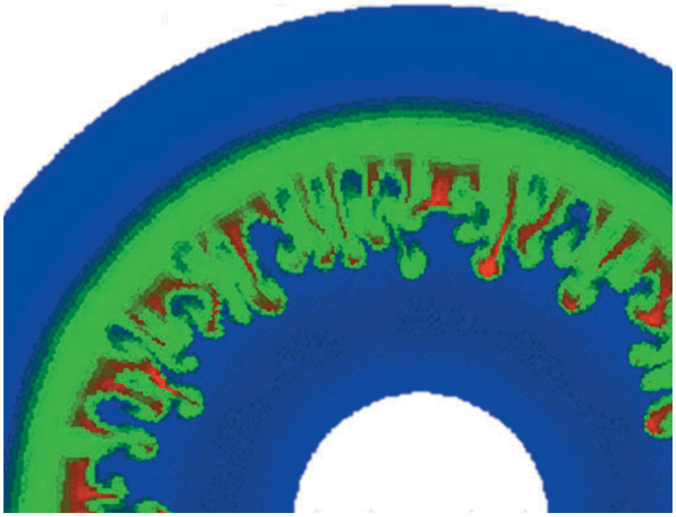
In 1992, President George H. W. Bush declared a moratorium on nuclear testing, and new weapons development ceased. The ending of the nuclear arms race dramatically affected the nation's three weapon laboratories—Livermore, Los Alamos, and Sandia—but their central missions still focused on national security science and technology.

In 1995, President Bill Clinton announced a new program called Stockpile Stewardship—an ambitious effort to improve the science and technology for assessing an aging nuclear weapons stockpile without relying on nuclear testing. For stockpile stewardship to succeed, all aspects of weapons must be understood in sufficient detail so experts can evaluate weapon performance with confidence and make informed decisions about refurbishing, remanufacturing, or replacing weapons as the needs arise.

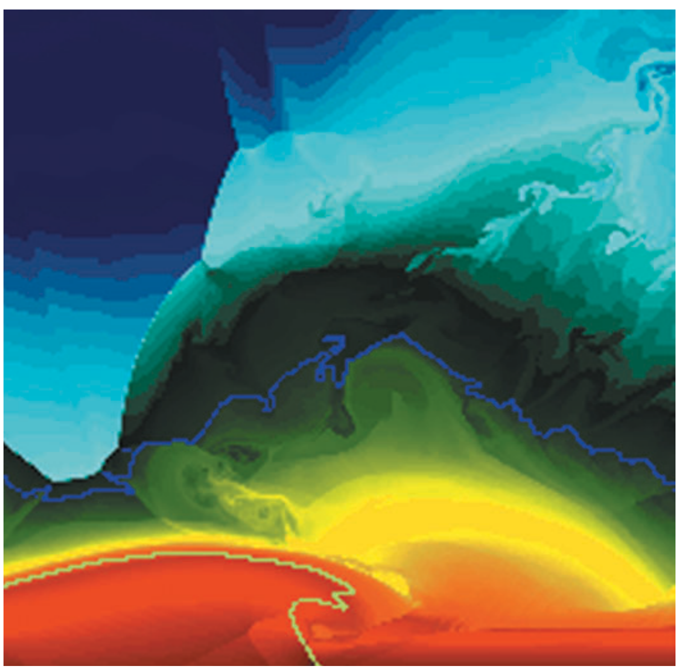
An Annual Assessment Review is conducted on the status of the stockpile. In this process, the secretaries of Defense and Energy receive formal evaluations of the stockpile from the three laboratory directors, the commander-in-chief of the U.S. Strategic Command, and the Nuclear Weapons Council. From those evaluations, the president makes a determination whether the weapons would perform as designed, should they ever be needed, or if nuclear testing is required again to certify performance. (See *S&TR*, July/August 2001, pp. 4–10.)

A view inside the target chamber for the National Ignition Facility (NIF), which is under construction at Livermore. Experiments with NIF will allow scientists to replicate various physical processes at the energy densities and temperatures approaching those in a weapon detonation. The first experiments are planned for 2003.

Aboveground diagnostic setup for an underground experiment at the Nevada Test Site. Data signals from a test explosion moved from the device, 300 meters downhole, up to the surface through cables, and the cables fanned out along the surface to trailers that housed instruments for reading the signals.



Simulation from a Laboratory-developed code run on ASCI Blue Pacific, one of the Advanced Simulation and Computing program's supercomputers at Lawrence Livermore. In this simulation, an arbitrary Lagrangian–Eulerian hydrodynamics code is used to model fluid motion as a function of increasing temperature, pressure, and density (or a Richtmyer–Meshkov instability) in an imploding inertial confinement fusion capsule.



Snapshot of a simulation run on ASCI Blue Pacific. This calculation modeled the density field of an x-ray burst on the surface of a neutron star. The yellow curve is the detonation front, racing across the stellar surface. The blue curve shows how the initial surface of the accreted atmosphere deforms.

Maintaining a safe and reliable stockpile without underground testing required a culture shift for the weapons program. "It changed the fundamental nature of our work," says Anastasio. "In the past, we asked ourselves whether a design would work. Now, with stockpile stewardship, we want to know when weapons fail. To certify reliability in this broader area, we must survey the state of a weapon periodically throughout its life cycle and try to predict when we'll lose confidence in its performance."

Stockpile stewardship was a radical departure for the weapons program in concept, but not in day-to-day activities. "Stockpile stewardship is an extension of how we were already doing business," Anastasio says. "Originally, in designing a weapon, Laboratory scientists would conduct tens of tests to put a weapon in the stockpile. But by 1980, we knew enough about how weapons worked that we could just test them at their performance margins. So we only conducted one to three nuclear tests before certifying a weapon. We also were developing simulation tools to answer questions that had been asked for decades. In effect, we were early pioneers of stockpile stewardship, even though such a program didn't officially exist at that time."

Keys for Successful Stewardship

The basic concepts for the Stockpile Stewardship Program were developed in the mid-1990s under the direction of Vic Reis, the assistant secretary for the Department of Energy's Defense Programs, with input from the Navigators Committee, a small committee of experts from the weapon laboratories. "We knew that certifying weapon performance without underground testing would be a hugely complicated task," says physicist George H. Miller, who represented Livermore on the Navigators Committee. "We'd need a much better understanding of the fundamental physics involved in a nuclear detonation if we were to determine when a weapon would fail."

According to Miller, the committee focused on defining the key features for a successful program of stockpile stewardship. "Experimental capabilities would be crucial. We'd need laboratories where scientists could scale nonnuclear experiments to closely match weapon physics conditions so they could examine properties at the microstructural level. We'd also need to dramatically improve the fidelity of our computer modeling capabilities, so we could more accurately simulate these complex interactions. And perhaps most important, we'd need a new methodology for certifying the judgment and credibility of future stockpile stewards."

From the Navigators Committee meetings and additional workshops led by Reis, DOE created a program that builds on the talent, resources, and capabilities available at the three weapon laboratories. Now administered by the National Nuclear Security Administration (NNSA), the Stockpile Stewardship Program integrates data from past nuclear tests with past and present nonnuclear tests, fundamental science and component-level experiments, surveillance of actual weapons withdrawn from the stockpile, and advanced simulations.

Previous highlights on the Laboratory's 50th anniversary have discussed the new facilities being built at Livermore in support of the Stockpile Stewardship Program. For example, the National Ignition Facility (NIF), a 192-beam laser designed to produce 1.8 megajoules of energy and 500 terawatts of power, will allow scientists to replicate various physical processes at the energy densities and temperatures approaching those that occur in a weapon detonation. (See *S&TR*, September 2002, pp. 20–29.) Miller, who is now associate director for NIF Programs, says, "In effect, NIF will allow us to break apart the physics of a weapon and examine the processes in isolation."

Experimental facilities alone would not provide a robust stockpile stewardship effort. To analyze the new data, scientists also needed vastly improved computer modeling capabilities so they could simulate a weapon in three dimensions from start to finish.

"Just to simulate the physical interactions that we understood," says Miller, "we estimated it would take computing speeds of 100 teraops," or 100 trillion operations per second—nearly 100 times the computer industry's top speed in 1994. "To develop that capability within one decade, we'd need to outstrip Moore's law." That is, Stockpile Stewardship could not wait for computer speed to double every 18 to 24 months—a computer industry standard first predicted in the 1970s by Intel Corporation's cofounder Gordon Moore.

To provide the necessary computing resources, DOE developed the Accelerated Strategic Computing Initiative (ASCI), a multilaboratory effort with strong partnerships in the computer industry designed to push computational power to the 100-teraops level. Now called the Advanced Simulation and Computing program and administered by NNSA, ASCI is producing remarkable results.

"We're seeing unexpected benefits from ASCI all over the scientific community," says Miller. "It's almost a new field—developing three-dimensional codes to run on the big computers, like the ASCI White machine here at Livermore. It's improving our scientific understanding in biology, chemistry, basic physics—every area of science." (See *S&TR*, June 2000, pp. 4–14.)

Miller believes NIF experiments, which are planned to begin in 2003, will also enhance scientific capabilities in many research areas besides weapon physics. For example, NIF will give astrophysicists their first laboratory setting for studying astronomy and should greatly improve their understanding of space physics. (See *S&TR*, May 2001, pp. 21–23.) "It's breathtaking science," Miller says. "Once again, we're reminded that when the federal government invests in high technology, there are surprising spinoffs that benefit the nation in many ways."

Training the Next Generation

As with Laboratory projects over the last 50 years, Livermore's stockpile stewardship work is a multidisciplinary effort, involving researchers from many directorates, including Defense and Nuclear Technologies, Engineering, NIF Programs, Chemistry and Materials Science, Computation, and Physics and Advanced Technologies. (See *S&TR*, March 2001, pp. 23–25; May 2001, pp. 24–26; July/August 2001, pp. 18–20.) Not only does the Stockpile Stewardship Program help the

Livermore's largest two-stage gas gun, which is 20 meters long. The gun's projectile flies down the barrel at speeds up to 8 kilometers per second and, upon impact, produces a shock wave millions of times the pressure of air at Earth's surface. Gas-gun experiments such as this one, which is being set up by technicians Leon Roper (left) and Keith Stickles, allow scientists to improve their understanding of the physics of shocked fluids and condensed matter—an important part of the nation's Stockpile Stewardship Program.

nation maintain its nuclear deterrent, but it is also helping Lawrence Livermore maintain its capability base to respond to future national needs. In particular, the program provides the technological challenges that scientists need to hone their problem-solving skills and build the scientific credibility that is a hallmark of the nation's weapon laboratories.

According to Anastasio, training the next generation of weapon scientists is imperative when the nation's nuclear deterrent is maintained in the absence of nuclear testing. "The test moratorium is 10 years old," he says, "and many of today's stockpile stewards have no experience designing a weapon or fielding a test. NNSA's Stockpile Stewardship Program is designed to help this generation of scientists gain the kinds of experience that we used to get with underground testing."

Multidisciplinary research is especially important for the program to succeed. By building new research facilities and computing capabilities, NNSA is combining experimental laboratories with computational laboratories so that physicists, code developers, engineers, and technicians can work in teams to solve stockpile-related problems. For example, ASCI code designers are working closely with physicists, chemists, material scientists, engineers, and others from the weapons program to validate the new codes used to model weapon physics. "We're working together to model real physics and to validate the codes against experimental data from our underground experiments," Budil explains.

NIF will provide the same cooperative research opportunities on the experimental end of stockpile stewardship. The power of NIF will allow scientists to perform weapon-relevant experiments in an aboveground nonnuclear environment. Nevertheless, setting up experiments and diagnostics will be an immense challenge, similar in many ways to preparing for a test at the Nevada Test Site.

"In the past, a designer's career record in the test program gave him or her credibility," says Budil. "For example, George Miller's opinions about nuclear weapons and how they work have the weight and credibility of his extensive experience. Without a test program, how does the Laboratory maintain its expertise and the public's confidence?"

To develop this experience and credibility, says Anastasio, Laboratory managers must allow scientists to once again follow the bold ideas that lead to innovation. "Livermore cannot become a risk-adverse institution if we are to maintain our creativity and flexibility in responding to the technical demands of national security. We must give scientists a chance to fail. We must let talented people put their technical reputations on the line—let them experience a few sleepless nights and confront the reality that an experiment might not work—so we can certify their credibility at making such critical decisions."

According to Miller, this need to challenge and test a scientist's judgment is one reason the nation has benefited from having competition between Lawrence Livermore and Los Alamos national laboratories. "When someone is diagnosed with a serious disease—a disease that, even with the best medical science, is still understood imperfectly—the patient wants to get more than one opinion." For the past 50 years, the nation has used this same approach with nuclear weapons. By having two independent weapon laboratories, the federal government has two sources of independent advice. And, Miller says, "Should the experts disagree—whether we're talking about medicine or weapon physics—

The U1a complex at the Nevada Test Site. The complex consists of several buildings and instrumentation trailers from which scientists can monitor experiments conducted underground. Today, the complex is used for subcritical experiments, which provide data to complement those from past underground nuclear tests.

it's possible that something is being missed." By building research facilities and new technology capabilities to be used by researchers at more than one laboratory, the Stockpile Stewardship Program ensures that the nation continues to have independent sources of expertise, each with credible histories in weapons research and the necessary research tools.

The Future of the Laboratory

Anastasio says that the future for Lawrence Livermore is both exciting and sobering. "September 11 reemphasized our mission. The nation is facing unprecedented security challenges. At Livermore, we must use our science and technology to build capabilities that serve the national interest."

As with the activities for stockpile stewardship, the Laboratory's role in research and development for homeland security is emerging from its ongoing work in nonproliferation and counterterrorism. "The scope of homeland security is daunting," says Anastasio. "The nation needs tools and technologies to prevent attacks, reduce threats, and manage the aftermath, areas we have long been working in to develop the relevant technical capabilities. Unfortunately, there's no silver bullet—no single technological widget—to solve this extraordinarily complex problem, and a layered, system-level approach is required."

An important part of this effort will be assessing the risks and balancing competing priorities while implementing solutions. In developing the nation's nuclear deterrent and maintaining the stockpile, researchers at Livermore have demonstrated the capability to work problems from end to end, and they build on this approach to problem-solving in projects for homeland security. "To focus our research in the right areas," says Anastasio, "we must understand not only what threats are facing the nation, but also what is needed to counter them." Researchers no longer focus solely on military applications for new technologies but rather are developing tools that can be used in various venues—from airports, hospitals, and post offices to theaters and sports arenas.

"We are developing real products that we can put in the hands of the end users," Anastasio says. "Once new technologies are developed, we'll transfer them to U.S. industry and then train the end users so these new tools can be deployed effectively."

Such activities are not new to the Laboratory. Many of Livermore's mission responsibilities and programs are relevant to homeland security and provide the Laboratory's scientists with an excellent overall perspective of the threats, technical opportunities, and user needs. "Homeland security will be an enduring national security mission for the Laboratory," says Anastasio, "With our successful track record of scientific innovation and technology development, we can provide effective solutions for this long-term endeavor."

Science and Technology in the 21st Century

Part of Livermore's 50th anniversary celebration has been to look at the future of science and technology in the context of national security and opportunities for the Laboratory. To foster this discussion, the Center for Global Security Research (CGSR) sponsored a 2002 Futures Project called "Science and Technology for National Security: The Next 50 Years—Pioneering the Endless Frontier," a series of workshops designed to examine the interactions and conflicts of science and technology, national security, and globalization. The CGSR workshops did not focus on predicting future technologies or national needs. Instead, participants were encouraged to identify the trends that intersect these three spheres of influence because the difficult challenges of the future will most likely involve issues at this interface.

Eileen Vergino, CGSR deputy director and cochair of the Futures Project, said, "Through these workshops, we not only wanted to examine the science and technology requirements imposed by national security. We also wanted to evaluate the inherent challenges and constraints to security that may be caused by science and technology breakthroughs and by globalization in the next 50 years."

One important goal of the Futures Project was to facilitate discussions between communities that rarely interact. Workshops included science advisors at federal agencies, fellows from the American Association for the Advancement of Science, other social scientists and experts in policy and national security, undergraduate honors students at Pennsylvania State University, and some of the younger scientists at Livermore, who may lead the Laboratory in the future. "We wanted to bring a lot of bright minds together and get them talking to each other," says Jay Davis, CGSR's first National Security Fellow and the other project cochair. "We asked a lot of questions and then gave the participants time to discuss the issues we brought up so they could examine problems and opportunities from multiple viewpoints."

Vergino notes that the terrorist attacks of September 11 serve as a cogent example of the interplay between the forces of globalization, national security, and science and technology. "Because of recent advances in communication technology, such as cell phones and the Internet, we can quickly correspond with people around the world," she says. "These new tools can also empower small, geographically dispersed groups, who can become a threat to national security merely by exploiting existing technology."

As a result, the U.S. can no longer focus its national security policy primarily on threats from one superpower or nation–state, as it did during the Cold War. Instead, it must plan for a complex world of competing smaller-scale threats, many of which can quickly inflict disastrous, long-term consequences.

"A serious concern where science and technology threaten security is bioterrorism or even an outbreak of a naturally occurring disease," Budil says. "And this threat is not only to the United States, but to the global community. With the ease of international travel we have today, a disease outbreak in one country can quickly spread across the world."

Workshop participant Robin Newmark adds, "Many aspects of our lives have changed since September 11, and as a nation, we're trying to sort out the conflicts that arise between implementing an effective homeland security policy and protecting the personal freedoms that we hold dear. In a very short time, we've learned to accept that we might be searched before we enter a sports arena or board a plane to visit our grandmother."

Newmark, who leads Livermore's Geosciences and Environmental Technologies Division, says research laboratories such as Livermore have an important role to play in addressing these new security issues. "For the short term, we can modify our current tools and apply them to the security problems. But we also need to find better technologies for addressing these issues. By asking difficult, open-ended questions, the facilitators at the CGSR workshops are helping us consider these problems from many viewpoints."

Finding solutions to technically challenging problems requires devoted attention over the long term, and for that, researchers must have stable funding. Vannevar Bush's model for government funding of basic science research has been used effectively since World War II. But Newmark asks, "What would happen to research institutions like Livermore if our funding sources change in the next 50 years? What if universities must rely on corporate sponsorships? We also must consider how these changes might alter the focus of our research and what opportunities they might bring."

Of course, advances in any science can have unexpected social costs, and participants in the CGSR workshops were asked to consider the ramifications of future research and development efforts. For example, says Davis, "If we were to cure cancer or

Example trends that intersect the three spheres of influence—national security, globalization, and science and technology—as identified by workshop participants in the Center for Global Security Research's Futures Project. The difficult challenges of the future will most likely involve issues that intersect the three spheres.

cardiac disease, what effect might that have on retirement plans and health-care programs? Can we envision a way to protect our economy? Furthermore, in an increasingly globalized world, do our efforts to stop research in a particular area, such as stem-cell research, serve to simply move that research to another country where we can no longer benefit from it or provide ethical guidance on its application?"

Budil adds that this kind of brainstorming, where participants not only contribute ideas but also evaluate the consequences of each choice, allows scientists to exercise their skills at making connections across disciplines—a skill that often leads to innovative uses of old technologies. "One of the great innovations to come from the Laboratory's weapons program is PEREGRINE," she says. (See *S&TR*, June 2001, pp. 24–25.) "Who would have guessed 20 years ago that we could spin off a tool for planning cancer radiation treatments by combining our expertise in Monte Carlo modeling and radiation transport? But those are the connections that scientists can make in a multidisciplinary environment such as this Laboratory, and the CGSR workshops encourage the discussions that lead to such connections."

The final workshop was held in September 2002, in conjunction with Livermore's 50th anniversary celebration, and a report on the Futures Project will be issued in the next fiscal year. Says Vergino, "It's clear from the discussions we've had that U.S. national security depends on maintaining our lead in science and technology. The nation must continue to support a strong, flexible capabilities base, as it has since World War II. To respond quickly in times of crisis, our government needs talented scientists and engineers—people who can understand complex problems, rapidly analyze scenarios, and then integrate systems to implement strategic solutions, whatever that might be." (For more information on CGSR, see *S&TR*, June 1998, pp. 10–16, and September 2001, pp. 11–18.)

According to Lee Younker, associate deputy director for science and technology, the greatest success of the Futures Project is that it stimulated the thinking of the participants. The project also helped Livermore's senior managers to refine their ideas for how the Laboratory's role might evolve over the next 50 years. "The defining events for the United States affect national priorities," says Younker, "and they often refocus the nation's attention on its science and technology infrastructure. National laboratories must be prepared to respond quickly in critical times by devoting people and resources to the research areas where they can have an immediate effect on problems of national importance."

Innovative Science Is a Moving Target

In its 50th anniversary year, Lawrence Livermore faces new challenges. Nuclear weapons remain part of the nation's security policy, but the number of weapons in the stockpile has declined dramatically. The nature of national security is evolving, and the Laboratory must follow that evolution to maintain its vitality. Thus, Livermore's senior managers must determine how the Laboratory can best contribute to its evolving security mission and which capabilities will complement other national needs.

Younker says that part of Livermore's success stems from the stable funding it has received for weapons research. "We're a superb laboratory when we have resources to do what we do best." In today's economy, few industries can afford to work on large-scale basic science research or technology development because they need a quicker return on their investment as determined by market forces. Federal funding of science and technology projects, such as nuclear weapons research or the space program, typically has a much longer-term horizon and thus has provided a tremendous benefit for the country. But Livermore's senior managers know the Laboratory must continue to evolve, as it has under the Stockpile Stewardship Program, so the institution and its capabilities base can remain a vibrant national resource for the next 50 years.

"We can predict the future all we want and be wrong," Miller says. "What's important is for the nation to have a system that provides capabilities and flexibility so the country can respond to whatever threatens us. We can't sit back and wait—our enemies will find a way to attack us if we remain static. Instead, we must use periods of relative peace, as we've had more or less for the last 50 years, to try to push our knowledge and technology in a positive direction and prepare for times of crisis."

"In one sense," says Anastasio, "the future of Lawrence Livermore is to be the thing we've always been, and that is a laboratory of outstanding people who can get work done—who are flexible, responsive, and make great contributions to our country."

—Carolin Middleton

Key Words: Center for Global Security Research (CGSR) Futures Project, nuclear test moratorium, post–Cold War science and technology, stockpile stewardship, underground nuclear testing, Vannevar Bush.

For more information on the Center for Global Security Research:
www.llnl.gov/nai/cgsrjd/cgsr.html

For Vannevar Bush's complete report, Science: The Endless Frontier:
www.nsf.gov/od/lpa/nsf50/vbush1945.htm

For further information about the Laboratory's 50th anniversary celebrations:
www.llnl.gov/50th_anniv/